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# **FINAL REPORT**

on BASIC RESEARCH IN ELECTRONICS (JSEP)



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In addition to the progress, we include for each of the work units the publications during the past year resulting from the research, and some of the recent interactions with the DoD or industry or other academic institutions. At the back of this Final Report we present our Report on Significant Scientific Accomplishments, and after that we append a comprehensive list of all the journal publications and conference proceedings during the period from August 1, 1980 to the present, arranged alphabetically according to the name of the first author.

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### **ABSTRACT**

This Final Report presents a summary of the scientific progress and accomplishments on research projects funded by the Joint Services Electronics Program (JSEP) for the contract period from 1 April 1980 through 31 March 1982. It does not contain information regarding accomplishments on research projects funded in other ways.

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### A. MILLIMETER WAVE WAVEGUIDES AND ANTENNA ARRAYS

Professors S.T. Peng, A. Hessel, and A.A. Oliner

Unit EM2-1

### 1. OBJECTIVE(S)

To systematically examine the properties of a class of periodically-modulated dielectric waveguides to assess their suitability as scanning antennas for the millimeter wave range. The study would involve first the analysis and measurement of several types of dielectric waveguides suitable for mm wave applications. The results would then be employed in an investigation of periodically-modulated leaky-wave structures for use as linear or two-dimensional antenna arrays. These antennas can have a low profile or be flush-mounted, are inherently rugged, are simple to fabricate, and can be made conformal to the surface of a moving vehicle.

This comprehensive investigation involves the solution of a number of constituent unsolved theoretical problems which are basic in nature and of substantial interest in their own right.

### 2. APPROACH

The antennas are viewed as leaky-wave structures and are analyzed by considering them as waveguides with a complex propagation constant; the propagation behaviors are determined by microwave network methods. For a systematic and thorough understanding of the wave processes involved, the complex waveguiding problem is broken into simpler constituent ones which are of great theoretical importance in themselves and can be handled independently. The overall waveguiding characteristics are then analyzed in terms of the wave processes associated with each constituent problem. In fact, the computer program for the grating antenna problem will consist of subprograms separately developed for each constituent problem.

### 3. PROGRESS

This research program is divided into two basic parts: the properties of open dielectric waveguides for millimeter waves, and new types of scanning antennas based on these waveguides. Since a proper understanding of the waveguides must underlie any careful investigation into the antennas, the major part of the waveguide investigation had to be completed first.

### A. Open Dielectric Waveguides

The first part of this study required the analysis of the scattering of a surface wave incident obliquely on a dielectric step. Such a step corresponds to the side of a dielectric waveguide, and this scattering problem is a basic element of the dielectric waveguide investigation when accurate and reliable values of leakage are sought. The guiding

of waves by a dielectric strip guide may be viewed as the multiple scattering of a uniform surface wave by the two step discontinuities forming the side walls of the strip guide. Thus, the scattering of a surface wave by a dielectric step discontinuity is a basic problem in the analysis of such dielectric waveguide structures.

The previously-published information on surface waves scattered by a dielectric step corresponds mostly to TE surface waves normally incident on the step. For that case, convergence is rapid, and no problems arise. Our needs correspond to oblique incidence of either TE or TM waves, where the two mode types couple to each other, and are no longer independent, as occurs for normal incidence. Due to the poor convergence that results, a very large number of modes is required in the mode-matching procedure that one must use.

Because of this need to employ very many modes in the mode-matching method when oblique incidence is involved, we developed an improved calculation procedure for handling a very large number of modes. This procedure is based on a recognition of the properties of the higher-order modes. The new method permits one to include many higher-order modes in the calculation without requiring a large computer memory core and a long computing time. In addition, the scattered mode amplitudes for the lower-order modes can be easily determined while including the effects of the higher-order modes.

The physics of the scattering of surface waves obliquely incident on a dielectric step is of interest in itself, and such a study was previously reported only briefly by us.<sup>2</sup> Our solution at the time was only approximate, but it contained all the physics. We found that the scattering is accompanied by mode conversion of TE waves into TM waves, and vice versa, so that an incident wave gives rise to reflected and transmitted waves of the opposite polarization; by a Brewster angle effect for TE wave incidence (it is for TM incidence when uniform dielectric interfaces are involved); and by electric field singularities that occur at the corners of the dielectric step due to the TM components of the field. An updated investigation using all modes was conducted during this period in parallel with the waveguide studies. A comprehensive paper on this work is planned.<sup>3</sup>

The next phase of this study involved dielectric strip waveguides for millimeter waves; the specific guides studied included rectangular dielectric image guide, "insulated" image guide (and dielectric rib or ridge guide, which is a special case in which the strip and the "insulating" layer underneath are of the same material), and inverted strip guide. These dielectric strip waveguides may be viewed as composed of two dielectric step junctions with a length of planar dielectric waveguide between them. Propagation along such waveguides may then be described in terms of a surface wave which bounces back and forth between the sides, or step junctions, undergoing "total reflection" at each bounce.

Let us first consider what happens when a surface wave on a dielectric layer is incident at an oblique angle on a step discontinuity.

As mentioned above, for a normally-incident surface wave the TE and TM modes remain independent of each other. For oblique incidence, an examination of the boundary conditions at the step junction readily shows that TE and TM modes necessarily couple to each other there. Thus, if a TM surface wave is incident at an angle, for example, some of its energy will be mode-converted into reflected and transmitted TE surface waves.

Many papers containing approximate analyses of these dielectric strip waveguides have appeared in the literature. All of these approximate theories assume that only one surface wave mode is present and that the geometrical discontinuities at the step junctions can be neglected. These approximate methods thus neglect the TE-TM mode coupling occurring at the sides of the waveguides, and they thus miss the physical effects discussed here. In particular, that coupling produces a leaky mode instead of the purely bound modes predicted by the approximate theories.

The physical situation that gives rise to leaky modes is summarized in Fig. 1. Without the TE-TM mode conversion at the sides of the waveguide, only the TE mode is considered to be present by the approximate theories. That assumption requires that the incident and reflected TE "rays" in Fig. 1 are above cut-off (propagating), whereas the transmitted "ray," in the outside region, is below cut-off (evanescent), and that no TM mode contributions are present. In the more accurate situation, where mode coupling is included. TM mode "rays" must be added, as seen in Fig. 1. Since we are depicting the situation for which the TM mode is dominant, the reflected TM wave inside is certainly propagating but the transmitted TM wave outside may be propagating or evanescent, depending on the geometrical parameters. In most cases, that wave will be propagating; when it is, as shown in Fig. 1, it indicates that energy in the TM polarization will be leaking per unit length along the waveguide, with the result that the propagation constant is complex, with a non-zero attenuation constant  $\alpha$ .

It is important to note that the dominant portion of the guided wave energy possesses TE polarization but that the leakage energy has TM polarization, in the form of a TM surface wave propagating away from the waveguide at some angle. In all other known cases of leaky modes, the leakage energy possesses the same polarization as the exciting energy. The class of leaky modes described here thus constitutes a new class of such modes.

A typical plot of the attenuation constant  $\alpha$  of the leaky mode as a function of the guide width W is shown in Fig. 2. For a purely bound mode, the value of  $\alpha$  would be identically zero (since we are neglecting material losses here). The non-zero value of  $\alpha$  is thus due directly to the TM wave outside in Fig. 1. We observe that the curve in Fig. 2 also shows periodic large dips, which are "resonances" or cancellation effects. These strong dips are due to the mode-converted TM wave in the inside region of Fig. 1, which also bounces back and forth between the sides of the waveguide. Thus, the mode-converted transmitted wave produces the leakage, and the mode-converted reflected wave produces the resonance dips in Fig. 2. These are severe physical effects, not

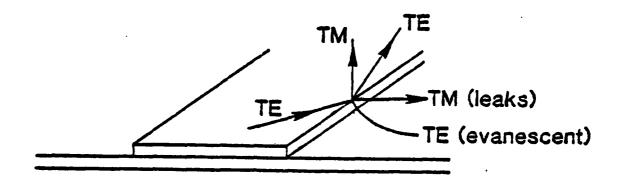


Fig. 1 Pictorial representation of mode-conversion effects at the side of a dielectric waveguide that give rise to leaky modes.

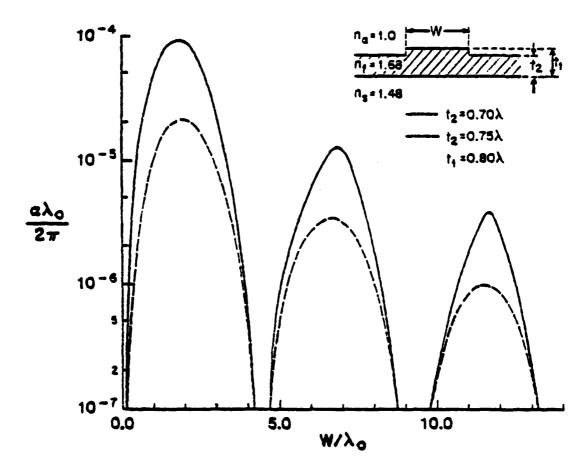


Fig. 2 Plot of attenuation constant  $\alpha$  as a function of guide width W for a rib waveguide fc integrated 1 optics. Note the periodic sharp resonance dips.

minor ones, and they are completely unexpected on the basis of the earlier published theories, which neglected the mode-conversion effects.

We have made calculations on most of the waveguides shown in Fig. 1. We have shown on fundamental grounds why the dielectric image guide for millimeter waves never leaks, and why most modes on the remaining waveguides will ordinarily leak. We have also found that the magnitude of the leakage may be large or small, depending on the type of waveguide, and we have shown why. We have also presented specific detailed examples for several of these waveguides. For example, the leakage is generally small for the inverted strip waveguide for millimeter waves, whereas it can become very large under appropriate circumstances for the insular guide. For a special case of the insular guide, the attentuation was as large as 4 dB per wavelength!

Our analyses and the physical explanations for these effects are contained in a pair of recent comprehensive invited papers<sup>4,5</sup> which keynote a special issue on open guided wave structures. We should also note a recent publication<sup>6</sup> by Japanese authors which describes an experiment they performed to detect leakage from a rib-type dielectric waveguiding structure. They make strong reference to our theoretical work and our physical explanation for the effect, and they conclude that their measurements verify the theoretical predictions.

Part of these studies involved examining when leakage would or would not occur, and for which modes, on the insular waveguide and on the inverted strip guide. The criterion used was developed first in the context of dielectric waveguides for integrated optics (reported in Work Unit EM1-4), and it was first applied there to rib waveguides. When adapted to the dielectric structure for millimeter waves, it was necessary to generalize the procedure. As a result, it has become a very simple, general method, essentially graphical, and based upon the easily-found dispersion curves for the separate TE and TM surface waves that comprise the elements of the final guided wave. A paper on this simple and systematic method is in the process of being written.

Our calculations for the inverted strip guide during the past year have shown that it is a versatile structure, in that the dominant mode can be made to be a TM mode or a TE mode depending on the geometrical parameters. If the dominant mode is TM, then the waveguide will not leak when excited in TM fashion, which is customary. When the dimensions are such that the TE mode is the dominant one, and the guide is excited in TM fashion, the guide can leak power contrary to expectations. We have made accurate and detailed calculations for the propagation characteristics, including the leakage properties, of inverted strip guide under a variety of conditions. We found that, depending on the geometrical parameters, the guide can leak in either the TE or TM mode, and that sometimes the leakage will occur for all values of strip width, and sometimes only for narrow strip widths. The behavior is predictable from the guide's geometrical parameters and from the dispersion curves for the inside and outside equivalent planar constituent regions of the waveguide's cross section. This phase of the investigation constitutes a portion of a Ph.D. thesis 3

We also set up a measurement program on leakage from dielectric waveguides, but much difficulty has been encountered with spurious radiation effects. The building of the set-up was completed some time ago, but unexpected radiation contributions have distorted the measured results. It is clear that leakage does occur, and in the proper polarization, and, in fact, part of the problem is that the leakage is so strong that multiple reflections of that energy are found. predicts that the energy should leak at a specified angle, and that, as one probes in a direction perpendicular to the guide axis, the leakage field should increase up to a critical distance and then drop off rapidly. We find that the angle agrees well quantitatively with theory, and that the transverse variation follows the theory reasonably well, except for interference effects which are quite strong. The primary source of the interference is a spurious space wave which emanates from the feed horn, and which seems very difficult to eliminate. These measurements do verify that the leakage obtained is indeed due to a leaky wave, is in the polarization expected, occurs at the right angle, and roughly corresponds to the expected transverse field variation. The strong interference, however, did not permit satisfactory quantitative correlation with theory for some of the parameters.

During the past year, we devised a novel alternative measurement approach, based on a <u>cavity resonance</u> procedure. Suppose the original dielectric waveguide is comprised of a dielectric strip on a dielectric layer on a ground plane, and that the strip extends in the z direction. We then place a length a of that guide between parallel vertical metal plates, where the metal plates extend in the x and y directions, thus forming a resonant cavity. In that cavity, between the plates, we then have a strip of dielectric of width a extending along the x direction, with its center portion, of "length" W, having a somewhat greater height since it corresponds to the strip of the original dielectric guide. If the mode on the original dielectric strip guide were purely bound, the fields in the x direction would be evanescent; if the mode were leaky, and a TE mode were incident, then a TM surface wave would leak away in the outside region.

The measurement approach employing the cavity now reverses the process. A TM wave is sent in from one end between the parallel planes, in the x direction, toward the central section of greater dielectric height, and the frequency is varied. If the condition for leakage were satisfied, the incident TM wave would excite a resonance in the central section, and the fields there would increase substantially, but only in the TE polarization (the inverse of the leakage situation). Hence, a probe sensitive to TE fields is placed just above the central section, and the power detected is found to peak sharply when the frequency of excitation corresponds to the condition for resonance. The fields scattered by such a cavity structure were also calculated theoretically and the agreement with measurements was excellent. Measurements were taken over a variety of strip widths and frequencies, and those measurements were compared with computations of the guide wavelengths and attenuation constants of the strip waveguides from which the cavities were created. Very good agreement was found between the

guide wavelengths and the resonance frequencies, on the one hand, and between the guide attenuation constants and the Q's of the cavities.

The novel cavity method verified that leakage indeed occurs, but it also offers a new method of measuring the leakage constant of these leaky waveguides. Resonant cavity methods have been used previously for the measurement of leakage constants of leaky modes, but the arrangement here is different. In other methods, a resonant cavity is created in the same way, by establishing metallic bounding planes, but there the guide section is excited longitudinally, via coupling holes in the metal planes. Here, the structure is excited transversely, by sending in the wave which would have leaked in the reversed situation. The details of this new measurement method, and the results of these measurements and their comparisons with theory, are contained in a Ph.D. thesis. 9

### B. Scanning Antennas Based on Dielectric Waveguides

In this program, we are concerned with scanning antennas for millimeter waves, where the antennas are created by producing gratings on the top surface of open strip-type dielectric waveguides. We have concentrated on the simplest of such waveguides, which is the rectangular dielectric image line, comprised of a rectangular dielectric block or strip on a metal ground plane.

The antenna structure we are analyzing first comprises a rectangular image line with a periodic array of grooves in its top face. Due to the periodicity, radiation of energy into space at some angle can occur. The antenna is analyzed by viewing it as a leaky waveguide (different from the previous leaky waveguides), where the leakage occurs from the top surface into space. We thus view the guidance of the mode in terms of surface waves guided by the corrugated, or grooved, surface, bouncing back and forth at an angle between the side walls of the guide, as shown in Fig. 3.

Thus, one must first know the propagation or guidance behavior of a surface wave traveling along a corrugated dielectric surface at an oblique angle with respect to the grooves. The case of a surface wave normally incident on such a grooved surface has been solved previously, but when the incidence is oblique to the grooves the problem is new, since now TE-TM mode coupling occurs, and the problem becomes a three-dimensional vector one. This vector problem was solved by us, and a computer program based on that exact solution was developed, and phrased in general terms. This solution or represents the first successful exact analysis of a three-dimensional vector boundary-value problem involving a periodic structure.

We have attempted to verify the accuracy of this solution by comparing its predictions with available experimental data, in two different ways. First, the computer solution was adapted to apply to corresponding corrugated dielectric surfaces for integrated optics, and then comparison was made with accurate measurements taken in Germany.

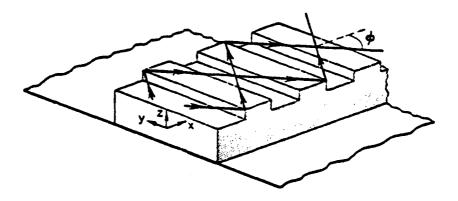


Fig. 3 Periodically-grooved dielectric image guide, showing guidance in terms of a pair of periodically-reflected surface waves.

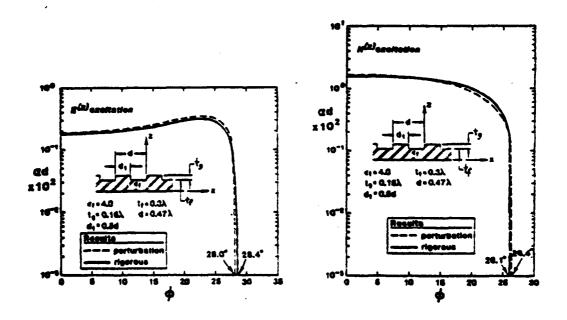


Fig. 4 The attenuation constant  $\alpha$  as a function of guide width (in the form of equivalent angle  $\phi$ ) for the lowest TM and TE modes on a heavily-grooved dielectric image guide.

Fig. 4(a), TM mode; Fig. 4(b), TE mode.

The agreement was excellent; further details are presented in Work Unit EM2-4, on optical waveguides.

The second way in which experimental verification is proceeding involves our own measurements at millimeter wave frequencies. We have constructed a waveguide comprised of a dielectric strip whose top surface is grooved periodically; instead of the sides left open, however, the grooved dielectric strip is placed between vertical metallic plates. The resulting arrangement is a trough waveguide, which is an approximation to the antenna itself, but for which we can calculate the propagation and radiation behavior exactly. In addition, accurate measurements are possible and spurious radiation may be kept low. We have already constructed the experimental set-up, and we have made measurements of the phase constant in the non-radiating passband. These preliminary results agree well with theory. Near the stop band, however, our early measurements show unsatisfactory pattern deterioration, but that region is always the most difficult one.

Many measurements have been taken on leaky wave antennas comprised of gratings on dielectric image guide, but no theory for the leaky wave behavior was available which takes the finite width of the guide into account. We have recently developed a theory  $^{11+12}$  which adapts the rigorous result mentioned above for oblique guidance by a grooved dielectric surface; it presents a straightforward procedure for determining the  $\alpha$  and the  $\beta$  of the leaky wave, thus permitting one to design such an antenna in accordance with desired radiation characteristics.

That design suffers in only one way, however. It is based on the rigorous theory for oblique guidance by a grooved dielectric surface, which is rather involved mathematically and therefore has an associated complex computer program. A practical design procedure should require a less involved computer program. Toward that end, we derived during the past year an <u>alternative and simpler procedure</u>, based on a perturbation analysis that yields simple closed-form solutions for the radiation characteristics of these periodic structures.

In this new analysis, the radiation of the surface wave in the presence of the periodic corrugation is formulated in terms of the radiation from an equivalent distributed dipole source. That source is due to the interaction of the surface wave with the periodic corrugation which is taken as a perturbation on a uniform (unperturbed) multi-layer dielectric structure. Such a method was originally developed by us for the special case of normal incidence, where the TE and TM polarized waves exist independently; many useful closed-form solutions were then obtained for the two polarizations separately. We have observed that the equivalent dipole source vector for the general case of oblique incidence may be decomposed into two orthogonal vectors, each responsible for the radiation of one polarized wave. Thus, the closed-form solutions previously obtained for the normal-incidence case can be simply employed for the oblique-incidence case, with only a slight modification of the TE and TM source amplitudes that account for the important effect of cross coupling between the two polarizations.

For best perturbation results, the propagation wavenumber  $\beta$  of the "unperturbed" surface wave must be chosen properly. It turns out that for TE mode incidence (when  $H_{\neq}0$  and  $E_{\geq}=0$ ), the value of  $\beta$  for the surface wave should be based on the volume average of the dielectric constant  $\epsilon$ , taking into account the tooth and gap regions of the grating. For TM mode incidence (when  $E_{\geq}\neq0$  and  $H_{\geq}=0$ ), the  $\beta$  value should be obtained from the volume average of the refractive index n ( $\epsilon=n^2$ ).

In order to check the accuracy of the perturbation expressions, a typical specific antenna geometry was selected and the numerical results obtained were compared with those found using the rigorous expressions. The value of the attenuation constant  $\alpha$  due to leakage was computed as a function of angle  $\phi$ , where  $\phi$  is shown in Fig. 3. The value of angle  $\phi$  depends on the guide width, being larger for narrower guides. These values of  $\alpha$  were computed at a specified frequency, but for both polarization excitations.

The first comparison, shown in Fig. 4(a), is made for vertical incident electric field polarization, corresponding to the lowest TM-like mode on a heavily-grooved image guide, which is the dominant mode on that guide. The solid line in Fig. 4(a) corresponds to the accurate but complex theory. Calculations derived from the new perturbation analysis are indicated by the dashed line. The agreement is seen to be very good, despite the simplicity of the perturbation expressions. In Fig. 4(b) the comparison is presented for horizontal incident electrical field polarization, corresponding to the lowest TE-like mode on the structure. Again, the solid and dashed lines represent the accurate and approximate results, respectively, and again the agreement is seen to be very good.

The very good agreement obtained between the solid and dashed curves in Fig. 4 indicates that the perturbation analysis yields rather accurate results. Since the resulting expressions for  $\alpha$  are in closed form and are relatively simple, this approximate procedure should also be a practical one for the design of this class of dielectric grating antennas for millimeter waves.

A summary of the theory underlying the new perturbation procedures was presented recently, <sup>13</sup> as was its application to radiation from dielectric grating antennas of finite width. <sup>14</sup> Additional details are contained in a Ph.D. thesis. <sup>15</sup>

Another important class of antennas for millimeter waves is the phase-frequency two-dimensional steerable arrays described in our proposal. Such arrays would be low-cost substitutes for the more-customary and more-expensive phase-phase scanning planar arrays. The phase-frequency structure is comprised of a periodic array of leaky-wave line sources, and is particularly suitable for the millimeter wave range. The analysis is made difficult because of the strong mutual coupling which is present between neighboring line sources, and it calls for a new approach along the lines of our proposal.

The overall structure is decomposed into unit cells with phase-shift walls, and then each unit cell is viewed transversely and seen to consist of sections. A fundamental section is that composed of a unit cell in an infinite medium made up of parallel dielectric rods, each rod of rectangular cross section. One must therefore find, as an intermediate problem, the dispersion characteristics and mode structure of the modes which propagate in such a rodded medium.

The problem of mode propagation in a rodded medium of that type is actually a basic, canonical problem in its own right, of interest in a number of antenna applications. In addition to its need in the phase-frequency class of dielectric antennas, it is directly applicable, for example, to two-dimensional phased arrays which have dielectric rods protruding beyond the ground plane for matching and bandwidth purposes.

The various steps required for the solution of this intermediate problem were described previously. Following those steps, we have determined the properties of all the modes of parallel dielectric slabs, including their orthogonality properties, and we developed suitable computer programs for them. We next obtained a transfer matrix for a dielectric rod of finite cross section, but of infinite length, and located in a unit cell with phase-shift walls, thereby accounting completely for all mutual coupling effects between neighboring rods in the medium. In establishing a computer program for this transfer matrix, however, we ran into a difficulty which we are in the process of overcoming.

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- 15. M.J. Shiau, "Scattering and Guidance of Electromagnetic Waves by Periodic Dielectric Structures," Ph.D. Thesis, Polytechnic Institute of New York (June 1983).

### 5. Dod and other interactions

- (a) Professor Peng spent two summers (1977, 1978) at the US Army CORADCOM at Fort Monmouth, New Jersey, working with Dr. Felix Schwering on dielectric grating and taper antennas, under an LRCP arrangement with the US Army Research Office. These interactions have continued in the form of a Post-LRCP contract and successor contracts.
- (b) Both Professors Oliner and Peng, but particularly Professor Peng, have held discussions (1979-1981) on electronically-scanned millimeter-wave dielectric grating antennas with Dr. Harold Jacobs of the US Army ERADCOM, Fort Monmouth, New Jersey, and have supplied information or the results of analyses on several occasions.
- (c) Professors Oliner and Peng participated in the millimeter-wave workshop sponsored by the US Army in October 1980 in Colorado; Professor Oliner presented a short talk on his JSEP-supported studies and was invited to be a member of the panel that evaluated the state of the art.
- (d) Professor Oliner has a contract with the Air Force's RADC/ET (Hanscom Field) on novel millimeter-wave antennas, but other than the grating structures studied under JSEP sponsorship.

### B. HYBRID RAY-MODE FORMULATION OF DUCTED PROPAGATION

Professor L.B. Felsen

Unit EM2-2

### 1. OBJECTIVE(S)

Ray optical and guided-mode expansions have been used as alternative methods for analyzing high-frequency propagation in layers and ducts. When the waveguide boundaries are penetrable, the discrete spectrum of guided modes is generally augmented by a continuous spectrum. In ducts of large cross section compared to the operating wavelength, the number of trapped modes may be exceedingly large so that truncation of the mode series has frequently been implemented, and the continuous spectrum ignored. Alternatively, ray models may require a very large number of reflected or refracted rays so that the "ray series" is terminated at some finite limit. Criteria justifying the truncation and assessing the resulting error have generally not been available. Numerical results for fields generated in this fashion may therefore be open to question.

In view of these observations, it is desirable to develop a systematic procedure that can account for the remainder of a truncated ray or mode series. A properly-chosen, range-dependent combination of rays and modes would not only furnish an accurate and convenient field representation, but would also provide new basic insight into the propagation process.

Our objective is to develop a new and systematic procedure that can account for the remainder of a truncated ray or mode series, and thus improve the accuracy of the field representation for high frequency propagation in layers and ducts. This is to be accomplished with a properly-chosen range-dependent combination of rays and modes, which also should provide new basic insight into the propagation process.

### 2. APPROACH

Field representation for propagation in layers and ducts in the high frequency range, where the field is generally characterized by very many rays or very many modes, will be determined by means of a suitably chosen mixture of both rays and modes in order to produce a more convergent and more accurate formulation.

### 3. PROGRESS

Numerical calculations have been performed for a variety of source-excited waveguides and ducts formed by two boundaries confining a homogeneous or transversely inhomogeneous medium. The hybrid ray-mode theory has been compared with reference solutions based on a normal mode (discrete and continuous spectrum) representation.

Calculations have been performed for the simplest case of a homogeneously filled parallel plane waveguide with impedance walls. They have also been done for open waveguides comprised, respectively, of a transversely homogeneous and of a transversely inhomogeneous layer above a semi-infinite homogeneous bottom. The former configuration was explored in connection with seismic propagation, and required extension of the hybrid method to transient fields. The latter configuration is of interest for sound propagation in an ocean channel with penetrable bottom. Here, the inhomogeneous refractive index was assumed to vary exponentially with depth; as noted previously, this model (by a simple coordinate mapping) also describes propagation along a cylindrically curved concave boundary in a uniform medium.

In all of the cases studied, the hybrid ray-mode formulation has exhibited the versatility and accuracy found in previous investigations of simpler problems. All of the problems are relevant to electromagnetic wave propagation in various environments (ground wave, tropospheric, optical graded index, circular waveguide) although some of them have been phrased in the context of wave propagation in other (acoustic and elastic) media. Thus, the hybrid method is now established as an effective tool for analyzing in a novel, numerically efficient and physically appealing manner source-excited propagation in multimode guiding regions. This assertion is supported by the various publications that have been prepared on this subject area, 1-11 and the basis has thereby been provided for application to even more general guiding regions with transverse as well as longitudinal inhomogeneities.

### 4. PUBLICATIONS

- 1. L.B. Felsen and A. Kamel, "Hybrid Ray-Mode Formulation of Parallel Plane Waveguide Green's Functions," IEEE Trans. on Antennas & Propag., AP-29, pp. 637-649 (1981).\*
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- 10. E. Topuz and L.B. Felsen, "High-Frequency Electromagnetic Fields on Perfectly Conducting Concave Cylindrical Surfaces," IEEE Trans. on Antennas and Propag., <u>AP-28</u>, No. 6, (November 1980).
- 11. E. Topuz, E. Niver and L.B. Felsen, "Electromagnetic Fields Near a Concave Perfectly Conducting Cylindrical Surface," IEEE Trans. Antennas and Propag., to be published.

### 5. Dod and other interactions

- (a) Two seminars on hybrid ray-mode methods for concave surfaces presented at ARO (Durham) 1980.
- (b) Three seminars presented during 1980-81 at U.S. Geological Survey, Menlo Park, California, on hybrid methods applied to seismology.
- (c) Collaboration with Dr. G. Jacobsen, Technical Univ. of Denmark, Lyngly, Denmark, on hybrid methods applied to beam propagation in optical fibers.
- (d) Collaboration with Dr. J.M. Arnold, Univ. of Nottingham, Nottingham, England, on hybrid methods applied to tapered dielectric waveguide.
- (e) Collaboration with Professor A.M. Scheggi, Institute for Electromagnetic Wave Propagation, Florence, Italy, on hybrid methods applied to optical fibers.
- (f) Collaboration with NATO Underwater Sound Laboratory, La Spezia, Italy, on hybrid methods for propagation in ocean channels.
- (g) Collaboration with Professor E. Topuz, Department of Electrical Engineering, Technical University of Instanbul, Turkey, on application of hybrid methods to imaging in multi-mode optical waveguides.

### C. WAVE-MATTER INTERACTIONS

Professors S. Barone, S. Gross and N. Marcuvitz

Unit EM2-3

### OBJECTIVE(S)

Our objective is to extend to nonlinear and/or higher power levels and to develop, both theoretically and experimentally, engineering expressions for "collision" (interaction) terms necessary in the description of particle-particle, particle-wave and wave-wave interaction problems arising in electromagnetic wave propagation through media in which ionization and related phenomena arise. The latter include microwave breakdown processes associated with high power wave propagation through the atmosphere, microwave propagation through and modification of the ionosphere, plasma screening effects in laser wave absorption and reflection by materials, etc.

### 2. APPROACH

An overall analytical theme is to obtain a kinetic basis for models of "collisional" interactions. Kinetic models must be consistent with the rate equations and the experimental rate coefficients and must provide reasonably correct representations of physical phenomena both at the kinetic and fluid levels. For example, a possible general form for the kinetic equation describing the density distribution function  $f_a(v,r,t)$  of particles of type "a" from which fluid equations may be derived is:

$$\frac{d}{dt} f_a = \nabla_v \cdot D \cdot \nabla_v f_a + \nabla_v \cdot A f_a + C_a(f_1, f_2, ...)$$

where D and A are diffusion and friction coefficients indicative of long range (particle-wave) collisions and Ca is indicative of short range collisions. While it is also possible to include some short range (particleparticle) collisional contributions in D and A, others involving transfer of non-infinitesimal amounts of energy and non-particle conserving collisions, such as ionization and recombination, must be included in the Ca term. Our initial collisional models are suitable only for kinetic equations that are isotropic in velocity or energy. However, in the presence of large applied electric field the isotropy assumption has limited validity particularly when electron velocities are larger than the thermal speed. The use of the microscopic kinetic approach of Klimontovitch, together with the renormalization and quasiparticle techniques, are being explored to remove the isotropy limitation. Moment or fluid equations derived from such kinetic models will be checked for consistency with experimentally determined momentum, energy transfer, ionization, etc., rates. The sensitivity of kinetic and/or fluid descriptions to various collisional models will be studied by developing and comparing analytical and numerical models of overall physical processes on our interactive graphic computer facility.

### 3. PROGRESS

### A. Introductory Remarks

General approaches have been developed for "collision" (interaction) terms required in the description of particle-particle, particlewave and wave-wave interaction processes which arise at those highpower levels at which ionization and related phenomena take place during the propagation of an electromagnetic wave through various media. The common underlying analytical theme has been to obtain a kinetic base for models of "collisional" interactions. Although the research has been applied mostly at laser frequencies, a general approach in terms of a quasiparticle treatment of wave propagation through nonlinear media 1-3 is also applicable at microwave frequencies. We have applied this approach to specific electromagnetic wave-media interactions such as ionospheric scintillation and turbulence, 4-8,24 laser propagation, 9-12 laser interaction with metallic and surfaces 13-19,23 and, to a lesser extent, high-power microwave propagation and breakdown. 20,21 Investigation of the basic interactions in different electromagnetic frequency regimes has been helpful in the development of both analytical treatments and computer models for comparison with experiment.

### B. Ionospheric Turbulence

A three-dimensional extension of our previously reported two-fluid theory of ionospheric plasma bubbles in the collision-dominated regime was completed in the past period. Effects of magnetic dip and the finite extent of the bubble along the magnetic field have been included. The theory clarifies the nature of the lifting force on a bubble. For closed bubbles which do not deplete an entire flux tube, two-dimensional theories are valid for bubbles having the smaller of observed transverse dimensions. For closed bubbles with the larger of observed transverse dimensions, or for smaller bubbles that do not extend most of the length of a flux tube, three-dimensional effects become significant. We find (1) bubbles rise more slowly than predicted by two-dimensional theories, (2) bubbles with different ratios of longitudinal to transverse dimensions rise at different rates, (3) bubbles which are not symmetrical about a meridian plane drift east-west. This is also a feature of two-dimensional theory which to our knowledge has not been previously noted.

Efforts to develop renormalization theory in a form suitable for the practical solution of ionospheric turbulence problems were continued. All known techniques can be viewed as approximations that strive to evolve a precise renormalization theory valid for strong (nonlinear) turbulence. Our work developed along relatively conventional lines, and also in directions indicated by renormalization group and divergent series techniques. During the past year, previous general results have been related to the direct interaction approximation in such a way that systematic improvements may be possible. This is one approach towards correcting some practical incompleteness in the direct interaction approximation for calculating the spectral index. We have made

some progress in carrying out this improved approximation in simple turbulent systems and in systems driven by stochastic fields.

One of the uncertainties in turbulence calculations revolves around the accuracy of the first term in renormalized perturbation expansions that are used to represent the statistical properties of waves propagating through the ionosphere. The accuracy is certainly in question for strongly turbulent ionospheres wherein the medium statistics impose radically different statistics on waves propagating through the medium. We have investigated the accuracy of a number of renormalization and summable divergent series procedures for expansions arising from different medium statistics and levels of turbulence. No definitive results have as yet been achieved. This difficult problem, which appears in a different context in the ionospheric turbulence work above, is generic to strong turbulence theory and has only been partially solved.

### C. Laser-Metal Interactions

Direct real-time measurements of a target material's optical properties with sub-nanosecond resolution may provide crucial, process-revealing signatures in following the interaction of an intense laser beam with a metal as the surface progressively undergoes heating, plastic deformation, slip, vaporization, ejection of liquid metal, plasma formation, etc. Three classes of physical processes have been proposed to account for a substantial decrease in reflectance observed during the interaction of an intense laser pulse with a metal surface: (1) deformation of the surface, (2) plasma formation, and (3) a non-linear process causing enhanced absorption within the metal. Thus far we may conclude that specular reflectance is a sensitive indicator of surface deformation. Total reflectance measurements, on the other hand, indicate that until the surface temperature of a metal target reaches the vicinity of the boiling point, the total reflectance does not differ significantly from that given by a Drude-type free-electron model. The reflectivity decrease of a Drude model for a metal heated from room temperature to a liquid at the boiling point is not large enough to account for the substantial reflectance decrease observed experimentally. 13 In addition to reflectance measurements, spectral measurements have begun on the plasma which forms in front of a copper surface at incident laser power densities above 3x108 W/cm2. Spectral emission lines have been observed from neutral copper atoms, ions and dimers (Cu<sub>2</sub>) in the plasma when the surface temperature of copper exceeds the boiling point. 18,23

Some of the basic phenomena which arise in the interaction of electromagnetic fields with metal surfaces have been examined. The major emphasis has been on the phenomena which occur during the formation of the hot layer of ionized gas near the metal surface. <sup>16</sup> The relationship between the growth of the laser-generated discharge and the time dependence of the plasma absorptivity was of particular interest because of the possibility of experimental verification. During the time period that the pulse power is near its maximum value, a large variation takes place in the density of the ablated material; thus the effect of thermal diffusion (via electrons) is important and is assumed

to dominate the effect of hydrodynamic expansion in determining cooling rates. The interaction process proceeds in a sequence of stages in each of which different phenomena take on primary importance. The various stages were isolated in our formulation for the purpose of analysis. These were (1) heating of the metal and formation of blow-off vapor, (2) heating of the vapor leading to breakdown, (3) propagation of the breakdown front and (4) build-up of higher stages of ionization in the already formed plasma.

In the analysis of the metal heating stage we presented a method of extrapolating existing data on material properties into the temperature range of interest. Because of the sensitive nature of the dependence of vapor pressure on temperature the results based on the extrapolated values differed significantly from those obtained by Harrach using a more approximate expression. A numerical integration of the nonlinear heat transfer equation led to surface temperature values substantially different from the predictions of the steady state model of surface evaporation.

The initial stages of the growth toward avalanche breakdown in the vapor proceeded in a way predicted previously when the spatial variation of the blow-off vapor density and pressure were ignored.<sup>22</sup> However, the time required for breakdown was substantially increased (doubled) over what was observed in the absence of the thermal diffusion terms. This term played a critical role during the avalanche process and during the subsequent propagation of the discharge front.

The propagation speed of the discharge front, in our model, was determined by the effectiveness of the thermal diffusion mechanism in equilibrating the electron temperature within, and in layers adjacent to, the discharge region. Thus the energy absorbed within most of the plasma goes toward the production of ionization in a spatial region in advance of the discharge front. During the propagation period, lasting several nanoseconds, the net transmission of the plasma decreases sharply as the absorption optical path length increases. The absorbed energy is stored in the ionized gas and is available for subsequent heating of the metal, possibly through emission of uv radiation.

Experiments by W.T. Walter, et al  $^{18}$  have been performed under conditions which correspond well to the assumptions of our model. Direct real-time reflectance measurements were made on copper targets irradiated with 30 ns pulses from a ruby laser. When the pulse intensity was around  $5\times10^8$  watts/cm² the observed reflectivity variation was in quantitative agreement with our results. Our studies also led to predictions on plasma temperature and state of excitation. These will be subject to experimental test when more complete measurements of neutral and ionized Cu lines are made in the "light flash" radiated by the plasma in front of the metal surface.

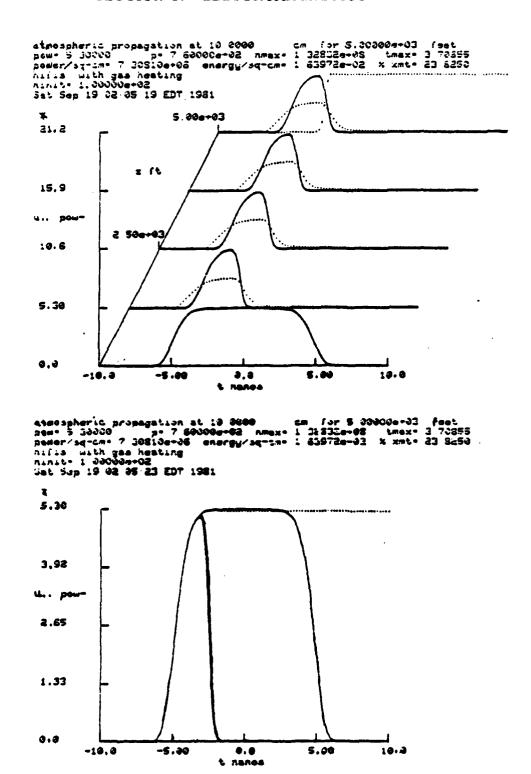
### D. High-Power Microwave-Atmosphere Interactions

The original model developed for the propagation of a high-power pulse has been expanded to include the temperature of the atmospheric gases and to allow for their heating by the propagating pulse. As we move from the shorter nanosecond pulses of interest for sneak-through propagation to longer microsecond pulses of interest for a dump of energy into a breakdown plasma, gas heating and hydrodynamic effects will play important roles.

The propagation of a 10-ns, 3-GHz pulse through 5000 feet at sea level, as obtained from our computer model, is illustrated in Figure 1. The peak power of  $7.3 \text{ MW/cm}^2$  is 5.3 times the power density required for dc or static breakdown (i.e., POW = 5.3). Pulse shapes at the antenna, one-quarter, one-half, three-quarters and full range are displayed by the solid curves along the z-axis in the upper portion of Figure 1. Dotted curves show the time dependence of the electron temperature at each range and the additional dotted curve at full range displays the time dependence of the electron density. The erosion of the tail during propagation of the pulse is more clearly illustrated in the lower portion of Fig. 1 where the five solid curves in the upper portion are displayed on a single xy plot (i.e., the outer solid curve is the pulse shape at z = 0 and the successively narrower solid curves are pulse shapes at quarter range intervals). At full range of 5000 feet only 23.8% of the initial pulse is transmitted and an electron density of 108 cm<sup>-3</sup> is produced.

To validate the microwave propagation computer model, we have assembled a conventional S-band rectangular waveguide system at the Polytechnic. A section of waveduige between two teflon windows is connected to a vacuum pump so that gas composition and pressure can be varied as desired. Air breakdown and pulse shortening are observed when the pressure within this waveguide section is reduced from atmospheric to a region in the vicinity of the Paschen minimum. In Fig. 2, for example, pulse shortening of a 30-kW, 80-ns, 3-GHz pulse is shown to take place when the pressure is between 1 and 4 torr.

Each experimental picture in Fig. 2 is a double exposure. One exposure shows the pulse transmitted in the partially evacuated wave-guide section when the waveguide pressure is reduced to the values specified under the picture. The second exposure shows the pulses transmitted when the waveguide contains atmospheric pressure. At 760 torr the field strength is too low to increase the electron density to a level where any modification of the pulse shape occurs. Also shown in Fig. 2 are the computer model results for propagation of a pulse at the specified pressures. Similar to the displays in Fig. 1, the solid curves show the pulse shape incident at the teflon window as well as after propagating 10, 20, 30 and 40 feet in the waveguide section with reduced pressure. In the results shown in Fig. 2, the actual experimental pulse shape was digitized into the computer and used in the model.



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Fig. 1 Propagation of a 3-GHz microwave pulse for 5000 feet through the atmosphere.

In Fig. 3 a similar comparison is shown for a 50 kW 400-ns, 3-GHz pulse. Pulse shortening is observed within a pressure region of 2 to 21 torr for this longer and higher peak pulse. Above 2 torr the agreement between experiment and computer model is good; however, below 2 torr the model results indicate erosion of the pulse tail, which is not observed experimentally. The comparison in both Figs. 2 and 3 has been improved by modifying the empirical coefficients used in the ionization coefficient  $\eta_i$ , the drift velocity  $v_d$  and the momentum transfer frequency  $\upsilon$ . In effect  $\eta_i$  has been divided by 1.3,  $\upsilon$  has been divided by 1.2 and  $v_d$  has been multiplied by 1.2.

A sensitivity analysis of the empirical coefficients has begun. The initial results indicate that the momentum transfer coefficient is the most sensitive. A 20% change in this coefficient produces twice the effect on pulse shape that a similar change in the energy to momentum transfer ratio coefficient or the average energy coefficient does. The ionization coefficient is less sensitive. A 20% change produces only half the effect on onset of pulse shortening.

Thus far, simple functional forms (linear, exponential, etc.) have been used for the empirical coefficients in the model. We have begun to examine the effect of utilizing closer fits of the empirical coefficients to the underlying data base. A modified momentum transfer coefficient decreased pulse shortening at all pressures. A modified energy/momentum transfer coefficient increased pulse shortening at all pressures. A modified average energy coefficient had little effect at the low pressure end but decreased the pulse shortening at the high pressure end. These modifications have not been incorporated into the model thus far. We may anticipate further changes in the empirical coefficients following an up-dating of the underlying data base.

Two additional processes must be considered in completing the validation: (1) the initial electron density to be used in the computer model and any residual-charged or easily-ionizable species remaining from a previous pulse, and (2) heating of the waveguide window producing initiators of breakdown. The experimental data in Fig. 2 were taken at a pulse repetition rate of 357; in Fig. 3 the rate was reduced to 8 pps. The initial electron density was 100 cm<sup>-3</sup> in the computer model results displayed in Figures 1-3. Substantial reductions (e.g., to 10, 1 or 0.1 initial electrons cm<sup>-3</sup>) do produce significant changes in the shape of the transmitted pulse. It is evident that additional work both theoretically and experimentally is required to complete the validation of the computer model.

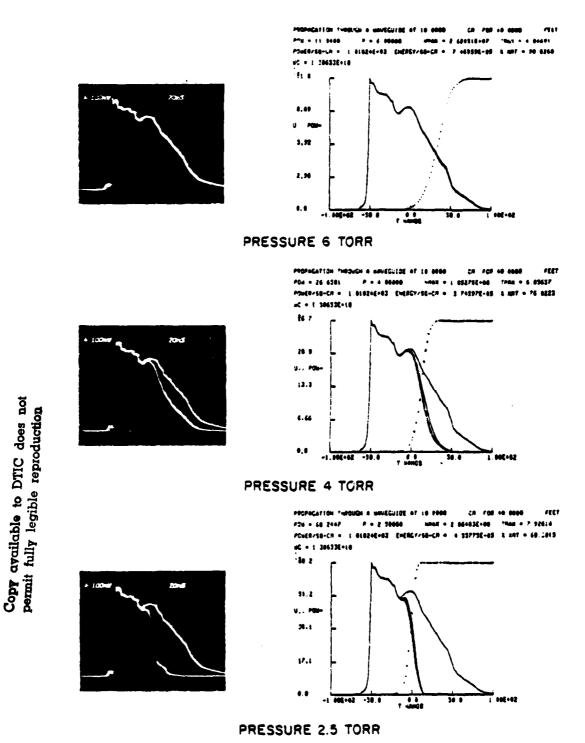


Fig. 2a Comparison of experiment with computer model results for propagation of a 3-GHz, 30-kW 80-ns microwave pulse in a partially-evacuated waveguide.

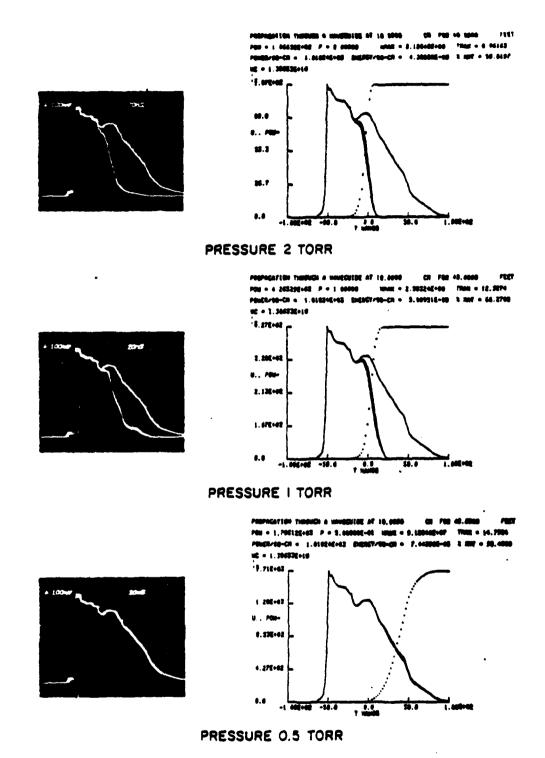


Fig. 2b Comparison of experiment with computer model results for propagation of a 3-GHz, 30-kW 80-ns microwave pulse in a partially-evacuated waveguide.

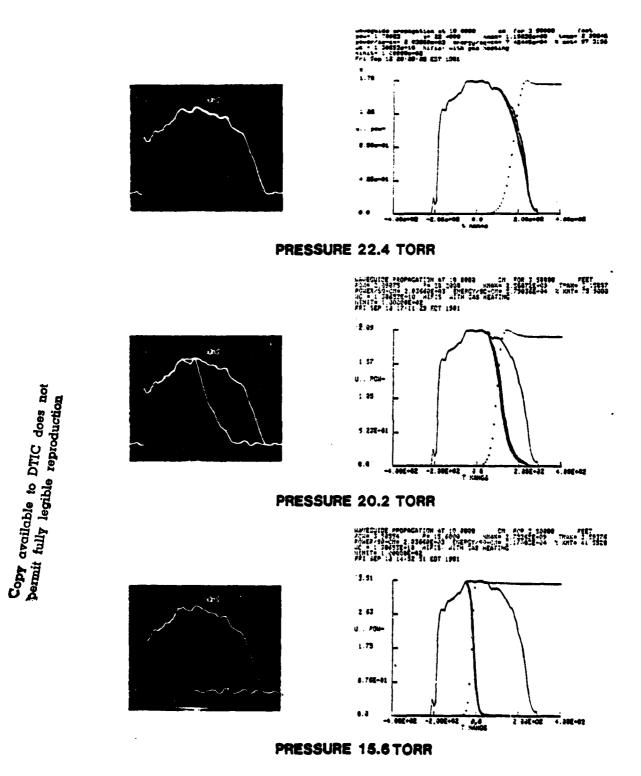
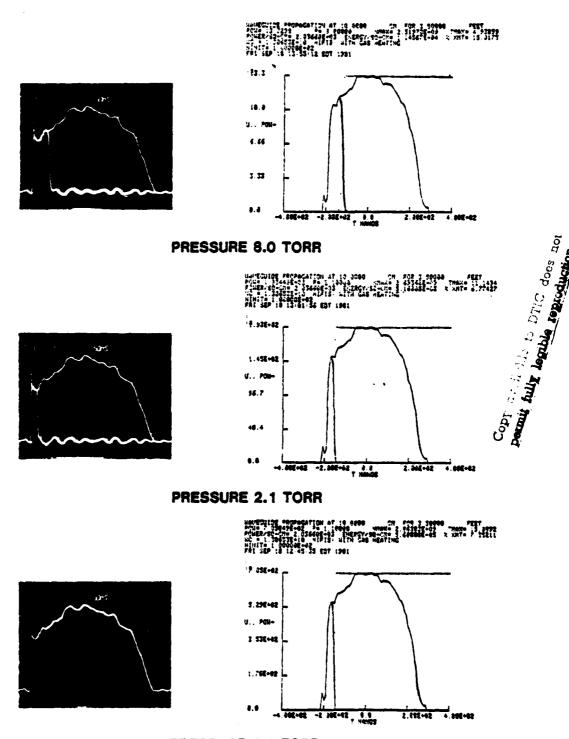


Fig. 3a Comparison of experiment with computer model results for propagation of a 3-GHz, 50-kW 400-ns microwave pulse in a partially evacuated waveguide.



PRESSURE 1.1 TORR

Fig. 3b Comparison of experiment with computer model results for propagation of a 3-GHz, 50-kW 400-ns microwave pulse in a partially evacuated waveguide.

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#### 5. Dod and other interactions

About three years ago, Professor Marcuvitz was contacted by R. Wasneski of NAV AIR about our willingness to investigate the possible realization of atmospheric channels created by and capable of propagating very-high-power microwaves for distances of a few kilometers. Such a possibility had been reported in a Russian publication. A quick NAV AIR sponsored study indicated that channel creation was not feasible with currently available microwave sources. Other possibilities, however, for the transmission of high-power microwave pulses were suggested during the study and have led to a continuing relationship with NAV AIR and NRL.

As a related consequence of this program, Professor Marcuvitz was invited to become a member of the recent special DoD committee to undertake the development of a preliminary plan for a U.S. High-Power Microwave Technology (HPMT) program with potential applications to DoD missions.

The background for our quick response stemmed from some of the basic nonlinear and turbulent wave propagation studies that originated from our JSEP research. More specifically, our program on this work unit provided basic technical contributions for our recent NRL-sponsored program on "High Power Microwave Pulse Propagation," which is both theoretical and experimental. The computer models resulting from this analysis and their low power experimental verification at MRI by Professor Walter are going to be checked with the gigawatt magnetron facility under construction at NRL. Modification of transmitted microwave pulse shapes, which have been examined at kW/cm² power densities at Polytechnic, can be tested at MW/cm² peak power densities at NRL and used to validate the computer model for microwave pulse propagation being developed at the Polytechnic. This is a cooperative project in which Polytechnic personnel and equipment will be moved temporarily to Washington, DC, to carry out the measurements together with the NRL personnel.

# D. OPTICAL WAVEGUIDING STRUCTURES

Professors T. Tamir, A.A. Oliner and L.B. Felsen

Unit EM2-4

# 1. OBJECTIVE(S)

- (a) To investigate the waveguiding and coupling properties of dielectric gratings having asymmetric (blazed) profiles for applications to beam couplers, filters, distributed-feedback lasers and other integrated-optics components. In particular, criteria for the design of high-efficiency gratings with prescribed desirable characteristics will be studied.
- (b) To analyze and characterize the behavior of basic discontinuity structures found in integrated-optical circuits, to determine their reflection and scattering characteristics. No one has yet performed such analyses to any degree of accuracy. The simple dielectric step junction will be examined first. It will be analyzed rigorously, and then to varying degrees of approximation, determining the simplest form suitable for recommendation.
- (c) To analyze the propagation characteristics of various linear (strip-type) waveguides of importance in integrated-optical circuitry. Most such waveguides have so far been analyzed by others only to first order. A better analysis has already revealed the presence in some waveguides of leakage and resonance effects which were heretofore unrecognized and which could have important device implications. Several different types of waveguide will be examined, and to various degrees of accuracy. The results obtained under (b) above for the dielectric step junction (since the sides of strip waveguides correspond to such junctions) will be applied in this connection.
- (d) To examine analytically the properties and the implications of a newly-recognized total absorption effect associated with thin lossy layers and with metallic periodic structures which are not perfectly conducting. Recent work has shown<sup>2,28</sup> that, if electromagnetic energy is incident on a planar structure consisting of a thin lossy layer and/or a metallic grating, all or nearly all of the incident energy can be absorbed by properly adjusting the incidence angle and the dimensions of the planar structure. The interesting aspect of this effect is that total absorption can be realized without the need for thick lossy absorbers. The aim of the proposed work is to first examine the total-absorption effect in detail for both layered media and periodic (grating) structures and then to consider the possible application of this effect in electromagnetics and optics.
- (e) To explore a new asymptotic theory for propagation in guiding regions with inhomogeneous permittivity properties. The results are expected to be relevant for integrated-optical and optical fiber waveguides, underwater sound wave propagation in the ocean, ducting in the ionosphere, and related applications. This theory will

be applied to various graded-index waveguides, including both slabs and fibers, with a view toward accommodating analytical refractive index profiles of arbitrary shape. Such structures would include profiles with discontinuous changes in the index or its derivatives; the theory will later be generalized to waveguides with asymmetrical boundaries, with longitudinal variation, and with curved axes.

(f) To examine the mathematical and physical implications of surface waves guided obliquely on periodic planar dielectric waveguides. When surface waves are guided perpendicularly to the periodic grooves, the mathematical problem is a scalar two-dimensional one in which TE and TM waves remain independent of each other. For oblique guidance, TE-TM mode coupling occurs and the problem becomes a vector three-dimensional one. This mode coupling results in a variety of physical effects that should be explored.

## 2. APPROACH

The approaches used in the various aspects of this program employ a number of theoretical techniques that have already been developed to a high degree of sophistication and success in the area of microwave engineering. In particular, the researchers on this program have personally contributed significantly to the development of these techniques, which include transverse resonance methods, various approximate and rigorous modal methods, and periodic structure theory. In most aspects of the program, the theoretical techniques themselves are developed further in the course of the investigations. This is especially true in connection with the investigations relating to graded-index guiding structures, where a new method embodying local evanescent fields with complex phase is employed, instead of the conventional asymptotic theories which utilize local ray fields or mode fields with real phase.

## 3. PROGRESS

# A. Dielectric Gratings for Integrated Optics

Our study of dielectric gratings for integrated-optics applications has continued prior work on periodic structures, which had involved the development of exact field solutions and their accurate numerical evaluation<sup>1</sup>, in general, and their application to the analysis and evaluation of beam-couplers<sup>3</sup>, in particular.

In this context, we have achieved the following results during the past 3 years period:

- (a) We developed approximate<sup>5-7</sup> and rigorous<sup>15,22</sup> methods to evaluate scattering by gratings having arbitrary profiles, which could be either symmetric or asymmetric.
- (b) By using the above approximate and exact methods, we examined desirable directional effects produced by suitably blazed gratings. In particular, we showed<sup>6,7,10-15,16</sup> that gratings with asymmetric

triangular profiles may theoretically achieve 100% efficiency in coupling an incident surface wave into an outgoing leaky-wave bean.

- (c) We verified the foregoing theoretical predictions by an experimental effort<sup>12-14</sup> which used a microwave model of an optical grating. Using a design based on simplified criteria we had developed<sup>10</sup>, this experimental effort demonstrated the feasibility of fabricating beam couplers having a measured efficiency of over 98%. The microwave modeling procedure was subsequently examined<sup>23</sup> for use in a wider variety of guided optical waves.
- (d) The relevance of the directional properties of blazed gratings was reported<sup>8,16,21</sup> in the broader constext of integrated-optics components. In particular, we observed that these properties hold over a relatively wide (+20%) bandwidth, and for relatively large changes in grating profile and/or other physical parameters. Thus, the effects due to fabrication tolerances or other imperfections appear to be minor<sup>23</sup>, so that dielectric gratings should find greater application in the near future.

# B. Scattering Properties of the Basic Dielectric Step Junction

We have been examining both approximate and highly-accurate analytical formulations for the dielectric step junction. That junction is of importance because it corresponds to the side wall of dielectric strip waveguides, and also because it occurs as an integral element of other structures for integrated optics applications, such as multiplexers and modulators.

With respect to the accurate formulation, we ran into the convergence difficulties encountered in the millimeter wave studies, and described under Work Unit EM1-1. The problems are analogous, since in optics the dielectric layer is placed on a dielectric substrate, whereas at millimeter waves one uses a metal ground plane instead of a substrate. The calculational details are different (as is the computer program), but the basic features are the same. We therefore used the new calculational method discussed in Work Unit EM1-1, and we obtained results with greatly improved convergence. With the computer program thus modified and improved, we are obtaining various numerical results for the scattering and mode conversion of surface waves occurring upon their oblique incidence on dielectric steps.

# C. Leakage Characteristics of Dielectric Strip Waveguides

Our studies on the propagation properties of three-dimensional dielectric waveguides for integrated optics were the first to demonstrate that under appropriate conditions some modes can leak instead of being purely bound, as was widely expected. Such leakage can produce cross talk between neighboring circuits and deteriorate performance. Furthermore, these leaky modes form a <u>new class</u> of leaky modes since the polarization of the leakage energy is opposite to that of the excitation energy, in contrast to all other known cases.

An invited paper<sup>31</sup> has been presented which discusses the characteristics of these new leaky modes, explains why leakage occurs, discusses how one predicts which modes are leaky, and presents some numerical results. Two other papers are in the process of being written, one stressing additional basic material and another on a simple graphical method for predicting when modes on rib waveguides will leak. We were recently invited to present a pair of papers<sup>32,33</sup> on guidance and leakage effects on open dielectric waveguides. Those papers were more general in scope, but they included the above-mentioned leaky modes on optical dielectric strip waveguides. The invitations were extended in recognition of the fundamental nature of the achievements associated with this program.

Originally, our numerical values for leakage were computed by including only the surface waves and their interactions, and neglecting the contributions from the continuous spectrum, which would change the numerical values somewhat but would not introduce any new physical effects or alter existing ones. Nevertheless, now that accurate results for the dielectric step junction are available (see the previous section), we have made use of those results to obtain accurate numerical values which include all modal contributions. We therefore obtained reliable and accurate results for those waveguides for which we previously had only approximate values.

A paper<sup>34</sup> by Japanese authors appeared in March 1979 which observed that our published results neglected the continuous spectrum; they then presented results based on an accurate, but still approximate, method for taking into account all modal contributions and solving for the leakage. They compared their results with our admittedly-approximate ones, and concluded that ours were too small by an order of magnitude. In their paper, they criticized the usefulness of our approximate procedure because of the large discrepancy. However, they later informed us that they found a numerical error in their results, making them smaller by a factor of  $(1.6\pi)^2$ , which is about 25. They published a correction 35 to their numerical values, and presented a new curve which shows much closer agreement with our approximate data, but they unfortunately did not remove their earlier critical statement. In any case, when we compare our new accurate results to their published ones, we find very good agreement except in the vicinity of the resonance, or cancellation, points. Our results show very sharp dips, whereas their dips are filled in substantially, because of the approximate method they used to compute the attenuation constant which yields the leakage.

Since our only real disagreement with the paper by the Japanese authors was the nature of the dips, we examined carefully the leakage behavior in the neighborhoof of these dips. During the past year, we found the following interesting set of results. When we took into account only the constituent transverse surface waves in the solution, the dips were rigorously found to be <u>nulls</u>. We discretized the continuous spectrum contributions, and then took into account only one additional transverse mode, as an approximation to the continuous modes. That small modification was sufficient to soften the null and

thereby produce only a sharp dip instead of a perfect null. Taking more transverse modes into account served to soften the null further, but the dips produced always remained very sharp. Accurate numerical calculations showed that the dips were about three orders of magnitude below the maximum in the curve of the leakage constant  $\alpha$  as a function of the strip width or the frequency. We conclude, therefore, that the resonance dips in the leakage constant are not nulls, but that they nevertheless are very sharp and deep. Our results for the complex propagation constant (which of course includes the attenuation, or leakage, constant) are obtained by directly locating the complex roots. On the other hand, the Japanese authors first located the real part  $\beta$  of the complex root accurately, and then, using that value for the real part, obtained the imaginary part  $\alpha$  by means of an accurate approximation. Their method, which is less direct and accurate than ours, was therefore able to yield very good results for α except in the neighborhood of the dips.

Our proof with respect to these dips proceeded in terms of a rigorous equivalent network comprised of ideal transformers representing the coupling elements, and transmission lines for each of the surface waves and the discretized modes corresponding to the continuous spectrum. At each stage, i.e., taking into account only certain modes, the input impedance was examined; when modes corresponding to the continuous spectrum were included, the input impedance was found analytically to contain a resistive part that could not be cancelled out, so that the dips had to represent incomplete nulls. This study forms a portion of a Ph.D. thesis to be completed soon.<sup>36</sup>

A recent paper<sup>37</sup> by two Japanese authors describes an <u>experiment</u> they performed to detect leakage from a rib-type dielectric structure. The shape of the measured loss curve, including two deep dips, bears striking resemblance to the calculated leakage curve; the numerical values differ because of material loss and coupling losses at the feed and detection ends, as the authors indicate. The authors conclude that their measurements verify our leakage theory.

# D. Anomalous Absorption Effects in Multilayered and Periodic Structures

This investigation of anomalous absorbtion effects had been initiated<sup>2</sup> by the observation<sup>28</sup> that total absorption can occur in a dielectric grating having small losses even though all of the incident energy would have been scattered back into free space if these losses were absent. While the proposed investigation had focused primarily on the strong absorption effect, our study has revealed that the process that leads to this effect also accounts for other interesting phenomena, such as large displacements and distortion of beams incident on layered and/or periodic media. The results we achieved on these aspects during the past 3-year period are as follows.

(a) By using rigorous analytical methods, we have verified<sup>9,15,27</sup> preliminary indications<sup>2,28</sup> that the anomalous absorption effect is

due to a wave interaction phenomenon, whereby the incident field couples energy to a leaky wave that can be supported by the structure. In this context, we have also shown that the phenomenon can then occur on multilayered configurations that need not necessarily include any periodicity.

- (b) We have confirmed our theoretical predictions of the strong absorption phenomenon by means of an experimental effort  $^{18,19}$ . By using a microwave set-up as an appropriate model, we have obtained nearly total (>99%) absorption at 10.5 GHz in a slightly lossy (tan  $\delta$  = 0.07) wood layer, which showed negligible absorption at frequencies that differ by more than 0.5 GHz away from that central frequency. This has been the first observation of such effects in multilayered media.
- (c) We have explored the possibility of using the anomalous absorption effect to improve the response of photodiodes by maximizing quantum efficiency while maintaining minimal response time. Our calculations for silicon photodiodes show that this possibility exists, but the conditions for its realization are very critical. A relaxation of such critical conditions could be obtained by imposing a periodicity on the diode configuration, but this necessitates further exploratory work. In a different context, we have shown<sup>24</sup> that the total-absorption effect can be applied to the design of optical filters having desirable critical stop-band characteristics.
- (d) We have developed a procedure<sup>20</sup> for exploring the total absorption effect in terms of a pole-zero analysis of the planar scattering coefficients in complex wavenumber space. While similar analytic tools have been used in the past in network-theory problems, this procedure is novel in the context of wave scattering phenomena. A preliminary application of this method has already provided the interesting result that the total absorption effect can be obtained in simple canonic structures involving not more than a single layer placed between two semi-infinite spaces, of which one is a substrate. More interestingly, the superstrate may then either be a denser or a rarer medium. The former possibility was the only one that had been previously known for practical conditions, but the latter possibility is by far more useful because it allows incidence from air rather than from a denser (additional) medium, such as a prism.
- (e) We have provided the basis for a qualitative and quantitative description 17,25-27 of the absorption phenomenon in terms of a large lateral beam shift of the Goos-Haenchen type. This lateral shift is due to the wave-interaction process that occurs when the finite (Gaussian) incident beam excites a leaky-wave field which forms part of the scattered energy. A particularly interesting aspect of lossy media is that, depending on certain critical physical parameters, the shifted beam appears in unexpected forms, such as in a backward direction and/or with strong distortion in its amplitude profile.

As indicated under items (d) and (e) above, the study of absorption effect produced by planar lossy structures (of either multilayered or periodic varieties) has shown that a whole class of phenomena makes further investigations worthwhile. Such additional investigations are particularly relevant because the properties of electromagnetic fields in the presence of losses have so far been paid relatively little attention. This study will therefore be continued under the new JSEP contract.

# E. Propagation in Inhomogeneous Waveguides by Evanescent Waves and Complex Ray Techniques

Difficulties occur when one attempts to generalize the evanescent wave theory, which has been shown to be highly successful from non-leaky modal propagation in longitudinally uniform, lossless graded index waveguides, to curved or longitudinally non-uniform configurations where leakage occurs. To better understand the leakage problem due to curvature, we have looked at the canonical problem of a two-dimensional cylindrically curved reactive surface layer or dielectric slab. In this event, exact solutions are available for comparison.

As is well known, a mode that is completely trapped in a straight waveguide begins to radiate on the convex side when the waveguide is curved. Loosely speaking, radiation takes place when the local phase velocity, which is less than the speed of light in the exterior medium near the surface, approaches the speed of light as the observer moves away from the surface. Phrased in terms of evanescent waves, the angularly propagating local evanescent plane wave fields become less strongly evanescent with distance from the waveguide surface. In the transition region to the radiative regime, their character changes from evanescent on one side to essentially non-evanescent (i.e., almost ordinary local plane wave or ray fields) on the other side.

It had been hoped that a perturbation approach to the straight non-radiating waveguide mode would lead to a correct description of the (small) leakage when the waveguide is weakly curved. A thorough study revealed that this is not the case. It is indeed possible to find corrections to the phase paths and phase fronts on either side of the transition region, but it is not possible to connect these uniquely across the transition region.

One way to avoid this difficulty is to employ complex rays, i.e., local plane wave fields with complex phase which, in a homogeneous medium, proceed along straight lines in a complex coordinate space. In curved geometry, complex ray fields are generated by complex caustics (surfaces of revolution in complex coordinate space) and, depending on the point of origin of a ray on the caustic, may represent fields in real space that are strongly or weakly evanescent. Thus, the disjoint family of evanescent waves produced by direct tracking in real space becomes connected across the transition region when described in terms of complex rays. Complex ray theory therefore unifies the class of phenomena associated with "evanescent tunneling" of a wave field to the radiating regime because of curvature of the initial (caustic) surface.

Once the complex ray fields have been determined, they may be interpreted in real space in terms of the physically meaningful local evanescent waves, and one may now chart the complete and unique phase fronts and phase paths of a leaky field. Numerical calculations have been made to exhibit these quantities for wave fields with varying degrees of leakage.

Having understood the ray fields generated by a complex caustic, we have then employed these fields to synthesize the guided modes that may exist on circularly curved waveguides with prescribed surface reactance or slab parameters. One now requires both outgoing and incoming ray fields with respect to the caustic to describe modal tunneling. Invoking ray field closure in complex space, analogous to the "transverse resonance" relation in microwave network theory, one determines the self-consistent caustic parameters for "source-free" propagation. These parameters yield the eigenvalues of the guided modes.

We may therefore conclude that complex ray theory provides the unifying tool for asymptotic analysis of modal propagation on curved waveguides. The analysis requires extension of the rays as well as the guiding surfaces into a complex coordinate space. The analytic continuation is unique, and complex ray tracing numerically tractable (for complex ray tracing applied to beam fed parabolic reflector antennas, see reference 38). When leakage is strong so that the transition region is near the surface, one must employ uniform transition functions. These can be determined from rigorous canonical prototypes.

Having understood the complex ray description for circularly bent waveguides, we have also sought to generalize these results to accommodate weak deviations of the guide axis from the circular case. We have found in preliminary studies that, in general, the permissible deviations are tied to the geometry and do not appear to scale with frequency; i.e., increasing the frequency does not permit larger deviations. This is in contrast to what is known for ordinary geometric (real) ray fields, where surface features must change slowly with respect to the local wavelength; thus, "strong" geometric changes are permitted for sufficiently small wavelengths. For complex rays, "locality" may exist in complex space but may translate into "non-locality" in real space. This observation has also been made in connection with evanescent wave and complex ray tracing from large apertures. 39

In summary, the investigations described above have unified the asymptotic treatment of modal propagation on curved waveguides, and have also clarified the difficulties encountered when one attempts to generalize leakage phenomena from canonical (circular) to non-canonical configurations. The lesson learned is that such generalizations, usually done by perturbation, must be approached with caution. More work needs to be done in this important problem area.

# F. Surface Waves Propagating Obliquely on Periodic Planar Dielectric Waveguides

We have these past two years made calculations on a structure not previously included in our three-year program because of the sudden availability of very accurate experimental data, and our development of a somewhat similar theoretical procedure in another context for millimeter waves. The topic is that of optical surface waves propagating at an angle on a periodically-corrugated dielectric layer on a dielectric substrate. Such structures, with obliquely-incident waves, have been finding increasing application lately in such components as multiplexers, filters, and mode deflectors for integrated optics.

The guidance of optical surface waves propagating in a direction normal to the grooves on a periodically-corrugated planar dielectric waveguide is well known, and various theoretical treatments are available. Such structures have been used in grating couplers and in distributed-feedback lasers, for example. The electromagnetic boundary value problem for this case is scalar, and TE and TM surface waves remain independent of each other. When the surface wave propagates at an oblique angle with respect to the grooves, the TE and TM surface waves are now coupled together, and the boundary value problem becomes a three-dimensional vector one. The problem is one for which an exact solution has not previously been available.

A corresponding guidance problem was developed as a basic intermediary step in the analysis of a class of millimeter-wave antennas in Work Unit EM2-1. It was originally intended there to employ the solution only in the range of parameters for which a single leaky wave is produced, consistent with the antenna application. In the optical case, the geometry is somewhat different, in that the metal ground plane must be replaced by a dielectric substrate, and the applications of interest are usually in the non-radiating region, especially near or in the stop bands.

There was originally no thought to apply the millimeter-wave antenna solution to the optical domain, but the redirection was stimulated by the appearance of accurate experimental data in the stop band regions. We first learned about these experimental results at a Workshop<sup>41</sup> and then further at an Optical Society Topical Meeting.<sup>42</sup> The speaker, Dr. Reinhard Ulrich of Germany, indicated that no accurate theoretical data were available with which he could compare his measurements, and that a suitable theoretical expression would be very valuable.

We therefore revised the expressions developed for the millimeter wave case by replacing the ground plane by the substrate, and then we appropriately modified the computer program. Detailed calculations were made for the dispersion curves corresponding to the specific structure measured by Dr. Ulrich, and the agreement between the measured and theoretical results were remarkably good. It is important to recognize that these calculations were made in and near the stop band regions, which are the regions most challenging to the theory since the space harmonics must appropriately pair off properly there.

These dispersion curves in the stop-band region show that, due to the TE-TM coupling, two extra stop bands appear. The implications of these extra stop bands were recently investigated by us in certain millimeter wave dielectric devices which operate in the Bragg reflection region to produce strong reflections with negligible radiation. The TE-TM coupling turns out to produce an extra (unwanted) transmission dip or reflection peak, and thus potentially to impair the device performance. The relevance here is that a paper on this study was recently presented which also includes the comparison discussed above between Dr. Ulrich's measurements and our theoretical calculations.

During the past year, we have extended this basic theory in a Our previous results permitted us to compute the new direction. propagation characteristics of these surface waves guided obliquely on a planar grooved dielectric waveguide for integrated optics. computations led to dispersion curves for the behavior of these waves. Mathematically phrased, the solutions obtained yielded the eigenvalues for these guided surface waves. The theory was now extended to include the  $\underline{\text{eigenvectors}}$ , in mathematical phrasing; that is, the solutions now also include the relative amplitudes of all the field components. The theory now permits us to determine polarization content of the complicated fields that result when the TE and the TM constituent surface waves become coupled at each step of the grating.

We have applied this extension of the theory to the case of groove spacing wide enough to permit the n=-1 space harmonic to become radiating; all the other space harmonics remain bound, however. When the surface wave is guided in the direction normal to the grooves, the polarization of the radiating space harmonic remains simple, the same as that of the incident surface wave. As that surface wave is rotated with respect to the grooves, corresponding to oblique incidence, the polarization content becomes mixed. Our calculations show that the TE-TM coupling that occurs to the oblique angle results in a surprisingly large amount of cross polarization. In fact, for the larger angles, an obliquely-incident TE surface wave, for example, can actually result in a radiating space harmonic which has more TM content than TE content. The polarization conversion that results is therefore a major effect.

These studies of polarization content are part of a Ph.D thesis to be completed soon.<sup>44</sup>

It is also of interest that further examination of our rigorous solution for the oblique guidance of surface waves reveals that a <u>rich</u> variety of physical effects arise as a result of oblique guidance, which are not present at all for normal guidance. Among these effects are anisotropy phenomena, beam steering, radiation of beams at peculiar skew angles, and other strong cross-polarization effects in portions of the radiation region. Some of these effects were presented by us in recent <u>invited</u> talks. 45,46

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- 38. P.D. Einziger and L.B. Felsen, "Evanescent Waves and Complex Rays," accepted for publication in IEEE Trans. Ant. and Propag.
- 39. F.J.V. Hasselman and L.B. Felsen, "Asymptotic Analysis of Large Parabolic Reflector Antennas," accepted for publication in IEEE Trans. Ant. and Propag.
- 40. S.T. Peng, "Oblique Guidance of Surface Waves on Corrugated Dielectric Layers," Proc. Internat. URSI Symp. on Electromagnetic Waves, pp.341B-1 to 341B-4, Munich, Germany (August 26-29, 1980).
- 41. Fourth Workshop on Optical Waveguide Theory, Noordwijkerhout, Netherlands (September 1979).
- R. Ulrich and R. Zengerle, "Optical Bloch Waves in Periodic Planar Waveguides," Topical Meeting on Integrated and Guided-Wave Optics, Incline Village, Nevada (January 28-30, 1980).
- 43. M.J. Shiau, H. Shigesawa, S.T. Peng and A.A. Oliner, "Mode Conversion Effects in Bragg Reflection from Periodic Grooves in Rectangular Dielectric Image Guide," Digest Internat. Microwave Sympos., pp. 14-16, Los Angeles, California (June 15-17, 1981).
- 44. M.J. Shiau, "Scattering and Guidance of Electromagnetic Waves by Periodic Dielectric Structures," Ph.D. Thesis, Polytechnic Institute of New York (June 1983).
- 45. A.A. Oliner and S.T. Peng, "New Physical Effects Due to Mode Coupling in Various Dielectric Structures," Goubau Memorial Session of URSI National Radio Science Meeting, Los Angeles, California (June 15-18, 1981). Invited Talk.
- 46. A.A. Oliner, "New Physical Effects on Open Dielectric Waveguides Due to TE-TM Mode Coupling," to appear in Proc. Seventh Colloquium on Microwave Communication, Budapest, Hungary (September 6-10, 1982).

#### 5. Dod and other interactions

- (a) Professor Peng spent two summers (1977, 1978), at the US Army CORADCOM at Fort Monmouth, New Jersey, working with Dr. Felix Schwering on dielectric grating and taper antennas, under an LRCP arrangement with the US Army Research Office. These interactions have continued in the form of a Post-LRCP contract and successor contracts.
- (b) Professor Peng is currently (1980) performing a task on waveguides for integrated optics for Dr. John Zavada of the US Army ARRADCOM, Dover, New Jersey, under arrangements made through the Battelle Memorial Institute.

- (c) We are discussing arrangements for a collaborative program with Professor R. Ulrich of the University of Hamburg-Harburg on the topic of new physical effects due to oblique guidance on optical grating structures, where we would do the theory and his group would perform careful measurements.
- (d) Collaboration with Dr. G. Jacobsen, Technical Univ. of Denmark, Lyngby, Denmark, is continuing on hybrid methods applied to beam propagation in optical fibers.
- (e) Collaboration with Professor A.M. Scheggi, Institute for Electromagnetic Wave Propagation, Florence, Italy, is continuing on hybrid methods applied to optical fibers.
- (f) The studies on optical beam couplers and infrared gratings have led to collaboration and interaction with Dr. P.K. Cheo's group at United Technologies, Hartford, Connecticut, to whom we have supplied analytical solutions and numerical data.
- (g) The use of blazing for optimizing the performance of periodic beam couplers, which had originally been proposed by us, has been explored by Dr. Hammer's group at RCA Princeton Laboratories and has stimulated other efforts for designing and fabricating such blazed gratings.
- (h) Comparisons of analytical procedures and numerical data on beam and periodic-structure problems have occurred on a continuing basis with Dr. Streifer of Xerox Corp., Palo Alto, California.

# E. EVANESCENT WAVE TRACKING - A NEW APPROACH TO THE ANALYSIS OF LARGE REFLECTOR AND LARGE APERTURE ANTENNAS

Professor L.B. Felsen

Unit EM2-5

# 1. OBJECTIVE(S)

To develop a new method for analyzing the radiation properties of large aperture and large reflector antennas, based on the local tracking of evanescent wave fields from the feed to subreflector(s) and main reflector and then to the far field, without intervening integrations over an equivalent aperture plane.

The radiation characteristics of large reflector and aperture antennas are analyzed conventionally by the method of physical optics or the Geometrical Theory of Diffraction (GTD). By these procedures, one may establish equivalent fields on the reflector surfaces or in an aperture plane, and then perform Kirchhoff type integrations to obtain the far field. These integrations, when done numerically, are costly and time-consuming. While GTD (with uniform corrections) may be employed to yield the near and far field directly for certain special configurations, this is not possible for strongly tapered illuminations.

To avoid the need for integration over one or several equivalent aperture planes, a new method, based on local evanescent wave tracking and on complex rays will be employed.

#### 2. APPROACH

The determination of the phase paths poses a principal difficulty in applying the evanescent wave method, especially for large distances from the initial surface. However, one may show that the phase paths at all ranges are approximately hyperbolic in the weakly evanescent region near the field maximum. For symmetrical field distributions with Gaussian amplitude taper, all phase paths in the paraxial region belong to a confocal elliptic coordinate system, and this statement is equivalent to saying that the paraxial evanescent field in real space is generated by a line source (2-dimensional field) or point source (3-dimensional field) displaced into a complex coordinate space. It is proposed to approximate amplitude tapers that depart from the symmetrical Gaussian shape locally by a Gaussian profile, thereby providing a global evanescent field generated by a complex caustic. The corresponding phase paths in real space would then still be hyperbolic but not confocal. This feature should systematize and simplify the tracking problem.

#### 3. PROGRESS

Referring to the previous proposal, it had been hoped that hyperbolic paths, which correspond to a particular "canonical" tapered

aperture distribution, could be matched <u>locally</u> to aperture fields that depart from the globally canonical hyperbolic form, at least in the (paraxial) weakly evanescent region near the maximum of beam-type fields. However, by comparison with independently calculated fields for various non-canonical aperture profiles, we have found that this is not generally applicable, although the procedure is adequate and advantageous for certain types of initial distributions. The deviation of the true phase paths from a hyperbolic shape can generally not be ignored for accurate calculation of the field.

The difficulties may be overcome by calculating the phase paths and fields via complex ray theory, which also describes the propagation properties of local plane wave fields with complex phase. Complex rays follow straight trajectories in a complex coordinate space. They originate on a complex initial surface with complex initial conditions generated by analytic continuation of the specified real initial data. An observable field is associated with the real-space intersection of a complex ray; the true phase paths of evanescent wave theory (EWT) correspond to those real-space intersections of complex ray fields satisfying the constraint of constant exponential amplitude. While ray tracing in a complex coordinate space is generally quite involved, the procedure does become tractable for "slightly complex" rays characterizing the weakly evanescent fields near the beam maximum. However, the complex ray fields per se, unlike the real-space fields of EWT, do not have a simple physical interpretation. It has therefore been concluded that complex ray theory should be regarded essentially as an algorithm for solving the EWT trajectory and field equations. combined complex-ray and EWT approach is tractable, both analytically and numerically, and furthermore describes the complete evolution of the field from the near zone to the far zone in terms of physically significant wave processes.

The basic EWT and complex ray studies outlined above have been presented in a manuscript that has been accepted for publication. To further test the validity of the conclusions from this investigation, the EWT-complex ray approach has been applied to the direct tracking of an initial beam-type field from the source plane to the far zone via an intervening reflection at a paraboloidal surface. Here, the complex ray tracing required extension of the initial conditions as well as the reflector geometry into a complex coordinate space. The success of the procedure for the single reflector problem is documented in another paper accepted for publication. <sup>2</sup>

# 4. PUBLICATIONS

- 1. P.D. Einziger and L.B. Felsen, "Evanescent Waves and Complex Rays," accepted for publication in IEEE Trans. Ant. and Propag.
- 2. F.J.V. Hasselman and L.B. Felsen, "Asymptotic Analysis of Large Parabolic Reflector Antennas," IEEE Trans. Ant. and Propag., AP-30 (July 1982).

# 5. Dod and other interactions

Collaboration with Professor R. Zich, Technical Univ., Turin, Italy, and Professor F. Hasselman, Catholic Univ., Rio de Janeiro, Brazil on evanescent wave and complex ray methods for large reflector antennas.

# A. X-RAY GUIDED WAVE ELECTRONICS

Professors B. Post and H.J. Juretschke

Unit SS2-1

# 1. OBJECTIVE(S)

To use the anomalous propagation of x-rays in good crystals for developing guided-wave modes with optimal properties in thick crystals; to apply these modes to both the study of the solid state of the host crystal and the coupling of x-rays to other waves within the solid; and to examine coupled-mode techniques to determine their suitability for refining structure determinations in crystallography.

Dynamical interactions of multiple x-rays within nearly perfect crystals are intended to lead eventually to special waveguides and components that can form the basis for possible future coherent x-ray circuitry. A second portion of the program involves the coupling of x-rays to other wave types, such as optical or acoustic waves, within the crystal. If the interactions prove to be sufficiently strong, these other waves can be used to modulate the x-ray beam, or to switch it from one state to another. Thus, the x-ray beam could be controlled electronically; otherwise, it would be necessary to turn the crystal mechanically to achieve the desired changes. The proposed program on x-rays thus involves a number of fundamental investigations which could make possible a systematic approach to x-ray circuitry.

# 2. APPROACH

Based on the dynamical theory of n-beam interactions of x-rays in crystals, and on the availability of good single crystals of ever increasing variety, we will carry out a combined program of theoretical exploration and experimental realization of the behavior of x-ray modes traveling along directions close to those specifying two or more Bragg conditions within the crystal. Since strong dynamical effects occur only within minutes of arc or less of these directions, the experimental methods require high spatial and energy resolution. Coupling to other types of waves will employ the general techniques of nonlinear optics already well-developed in other frequency domains.

#### 3. PROGRESS

# A. Improvements in Instrumentation

- (1) The new 5kVA x-ray generator has been set up for very high intensity output, using special filaments, and it has been fitted with a grooved crystal Ge monochromator that has reduced the incident beam divergence to about 10 seconds of arc.
- (2) For Renninger type experiments, where the divergence must be small in any direction, we have set up pin holes about 1 m from the 0.1 by 0.1 mm target to obtain less than 30" divergence.

- (3) The use of divergent beams transmitting x-rays through the crystal in order to locate readily regions of many beam interactions, using the same type of target as in (2), has reduced the observation time on the rotating anode generator by a factor of 10 relative to the previously used stationary microbeam target.
- (4) We have acquired a Cr rotating target to extend the high intensity range of the instrument to other wavelengths.

# B. N-Beam Interactions

- (1) Efforts to extend phase determination from simple relatively perfect crystals<sup>1,2</sup> to mosaic organic crystals have not been successful, when Cu K radiation was used. Phase effects are there, but smear out. The use of Cr seemed to help. It increased the absorption by the specimen and, as discussed in the last report, such increases facilitate the observation of dynamic effects on the phase. Nevertheless, it appears at present unlikely that the use of Cr will make possible routine exploration of the phase determination. Still longer wavelengths would be needed, and for that we will use synchrotron radiation, probably at Brookhaven.
- (2) Studies of polarization effects in 3-beam diffraction have been completed.<sup>3</sup> This will be included in a comprehensive review of 3-beam diffraction to be published in Z. für Naturforschung, in early 1982.
- (3) We have collaborated with a group at the University of Amsterdam in a study of the relative merits of calculating phase probabilities based explicitly on dynamical diffraction theory compared with statistical methods now widely used. This study indicates that, even in its present primitive form, the dynamic approach is as successful in predicting probable phases as are these other methods. Results of this work are being prepared for publication in Acta Cryst.
- (4) A modification of our experimental approach to phase determination has been tried recently. It shows great promise for the determination of phases. In essence, it involves the application of the methods developed at the Polytechnic to the analysis of the intensity distribution of simultaneous reflections, but now recorded in the Bragg mode, under conditions of high resolution. The technique is simple and rapid. It has been successfully applied to the analysis of patterns of several simple substances. Work is proceeding to optimize the procedure and to apply the method to the determination of phases in mosaic crystals. The restriction of phase determination to cases where all structure factors involved are essentially of equal magnitude does not apply to the newer procedure. Any range of F's is usable.

# C. Interaction of X-Rays with Other Waves

The progress in understanding the dynamic interaction of x-rays with phonons, or with the phonon portion of polaritons in polar crystals, has been very satisfactory. The major new advance has been in treating this problem as an x-ray fully interacting with many

phonons. This approach is obviously needed when dealing with a thermal phonon distribution, but it was also found to be essential for the interpretation of an experiment of x-rays coupled to intense "monochromatic" phonons. In both cases, the n-phonon problem still reduces in practice to a set of n one-phonon problems, as far as the satellites are concerned. However, the line shape and the amplitude of the main reflection are influenced simultaneously by all phonons, and can be drastically altered. It is this discrepancy between observed and calculated intensities of the main reflection, already alluded to in the last progress report, that has delayed the publication of the two papers that have been in preparation.

The specific areas of progress are:

- (1) We have found a fully analytic solution of the six-beam case of an x-ray interacting dynamically with monochromatic phonons of intensity which may be small or large moving parallel to the reflecting planes of the crystal. In this formulation, the problem factors into cubic and quadratic equations, and gives explicit solutions for the three-sheet dispersion surface and the sixtuplets of x-ray field amplitudes associated with each point on this surface. We can therefore solve the boundary problem exactly, and determine explicitly all external reflected fields, for arbitrary intensity of the phonon beam. This exact solution has been extremely useful in exploring the consequence of changing the various parameters in the problem, and especially under what condition the usual weak coupling approximation holds. We have studied solutions of both model problems and of the specific interaction of Mo K-radiation reflected from the (004) planes of InSb.<sup>7</sup>
- (2) We have formulated the dynamic n-beam phonon problem, and set up the explicit equations for the 2n+1 sheeted dispersion surface, and all the associated fields. The procedure follows closely the method of item 1. Introduction of the boundary conditions leads to a 2n by 2n determinant for the relative incident fields, and also to the corresponding expressions for the reflected fields. When the coupling is weak, these results can be cast into explicit modifications of the uncoupled solutions for all but the main reflection. This reflection has to be solved using a modified dispersion relation. Our expressions show so far that this modification contains parts equivalent to the Debye-Waller factor, but also other contributions that appear only when the full dynamical problem is considered before making the weak coupling approximation.
- (3) We have evaluated the modification of the main reflected intensity for many thermal phonons, when the reflection occurs away from the Bragg angle, and find that the multi-phonon coupling leads to a significant reduction from that expected for the uncoupled two-beam case, or the case with the traditional correction for thermal diffuse scattering.<sup>8</sup> Numerical calculation is now in progress to determine this reduction quantitatively.

- (4) Reanalysis of the experimental results of the x-ray intense phonon beam interaction in InSb in light of the exact solution of item 1, above, has shown that the phonon beam used was, in fact, far from monochromatic, but had a spread in energy larger than that of the original Bragg peak, although its direction was still well defined. We have obtained specific expressions for the influence of this phonon distribution on the main line, where experimentally the intensity was seen to be reduced by 5 to 20%.
- (5) The interaction of x-rays with laser-induced polaritons in polar crystals has been analyzed from the point of view of energy transfer, and it is found that under optimal conditions, using normal laser intensities, the weak coupling approximation for the phonon part of the polariton is justified. This has made it possible to adapt directly the formalisms worked out under 1, above, to single phonons traveling in arbitrary directions, but with the additional condition that energy transfer between polariton and x-ray is not negligible. This implies that the coupled modes contain fields of differing frequencies, that refer to different dispersion surfaces. However, our formalism lends readily to incorporate this complication. One immediate consequence is that the expected six-beam coupling reduces to four-beam cases, i.e., polaritons are predominantly either absorbed or emitted, but not both. We are in the process of determining the optimum experimental configuration for observing the predicted laser-induced switching of x-rays at different laser frequencies.

The work reported here under items (1) to (5) represents a Ph.D. thesis in progress that is expected to be completed during the spring semester of 1982.<sup>6</sup> Various parts of this thesis will be prepared for publication.

# 4. PUBLICATIONS

- 1. B. Post, Acta Cryst. A 35, 17 (1979).
- 2. P. Wang, "Direct Experimental Detection of X-Ray Phases from Intensity Measurements," Ph.D. Thesis, Polytechnic Institute of New York (1979).
- 3. T. Hom, "Three Beam Dynamical Interactions," Ph.D. Thesis, Polytechnic Institute of New York (1979).
- 4. P. Gong, "Phase Determination from X-Ray Intensities," Ph.D. Thesis, Polytechnic Institute of New York, in progress. Also papers M6 and M7 presented at the American Crystallographic Association General Meeting at Gaithersburg, MD (March 1982).
- 5. S.D. LeRoux, R. Colella and R. Bray, Phys. Rev. Lett. <u>35</u>, 230 (1975).

- 6. F. Wasserstein-Robbins, "X-Ray-Phonon Interaction as a Dynamical N-Beam Problem," Ph.D. Thesis, Polytechnic Institute of New York, in progress.
- 7. H. J. Juretschke and F. Wasserstein-Robbins, "The Role of X-ray Boundary Conditions and Other Effects in Strong Dynamical X-ray Phonon Interactions", accepted for publication in Physical Review B.
- 8. F. Wasserstein-Robbins and H.J. Juretschke, "Dynamic Effects in X-Ray Thermal Phonon Interaction in Symmetric Bragg Reflection," to be published.

# 5. Dod and other interactions

- (a) The American Crystallographic Association will hold a special session honoring Professor Post's contributions to crystallography at the Spring 1982 meeting at Gaithersburg, MD. Both Professor Juretschke and Professor Post have been invited to present papers.
- (b) Some of the above proposed work may involve specific collaboration with laboratories in Brazil (Professor Chang), Greece (Professor Alexandropoulos), and Australia (Professor Wagenfeld). The collaboration is being proposed by them in order to participate in our research.
- (c) Professor Post has been presenting invited talks on aspects of the problem of phase determination in Amsterdam, Oslo and Trondheim, during the summer of 1980. He also presented a paper on the statistical aspects of phase determination, discussed above, at the meeting of the American Crystallographic Association, Ottawa, in August 1981.

# B. INTERACTION OF MILLIMETER WAVES AND SEMICONDUCTORS

Professor B. Senitzky

Unit SS2-2

# 1. OBJECTIVE(S)

The object of this study is to investigate the interaction of millimeter wavelengths with mobile charge carriers in semiconductors.

The effect of conduction carriers on guided energy is characterized by a complex dielectric constant which, in appropriate structures, attenuates and/or changes the phase of the guided radiation. This principle is the basis for the familiar class of devices which includes modulators, phase shifters, and switches. It is therefore important to have a quantitative understanding of the interaction of millimeter wave radiation and the non-equilibrium charge carriers which are injected from the terminals. In addition, it is also important to understand the interaction of the equilibrium charge carriers with the millimeter wave radiation since this will determine the electromagnetic properties of the active structure in the absence of injected carriers.

At present, the commonly accepted approach is to estimate the dielectric constant by assuming a simple Drude model with a single collisional relaxation time which is determined from DC resistivity vs. concentration characteristics. The validity of this assumption has been questioned both theoretically and experimentally, at microwaves and infra-red, but not at millimeter wavelengths. It is our primary goal to investigate, both theoretically and experimentally, the interaction of radiation with free carriers in semiconductors at millimeter wavelengths.

# 2. APPROACH

Our original approach was to study the interaction of millimeter wave energy and semiconductors in a slotted metallic waveguide. Because of the very small sizes involved, and the influence of discontinuity structures that extended the fields into regions outside the waveguide, this approach failed to yield reliable results. We are now studying the interaction by measuring the reflection and transmission properties of silicon wafers in free space with transmitting and receiving horns.

#### 3. PROGRESS

Let us first recall that semiconductor material is used to guide and control millimeter wave radiation. The millimeter wave energy is guided in devices such as waveguides and antennas, and controlled by switches, electronic phase shifters and modulators.

The control of the millimeter wave energy by semiconductors is usually achieved by changing the number of conduction electrons or holes in the electromagnetic field. In most applications the guiding

structure for the electromagnetic energy is designed so that the radiation can interact effectively with the semiconductor. At microwave frequencies, matching sections have been developed which can achieve the required interaction. At millimeter wave frequencies the matching structures become lossy, and factors such as junction capacity, lead impedance, and encapsulation further degrade device performance. New types of matching structures and semiconductor devices must therefore be developed for this frequency range. To accomplish this, a knowledge of the complex dielectric constant of the semiconductor as a function of the mobile carrier density is required.

Before proceeding, it is important to note that a unique dielectric constant can only be defined under certain conditions. Mobile charge carriers can have an equilibrium or non-equilibrium energy distribution. For example, carriers which arise from a background impurity level and are subject to a weak electromagnetic field are in an equilibrium distribution and can be characterized by a unique dielectric constant. On the other hand carriers which are injected by an electric field from external contacts are, strictly speaking, not in thermal equilibrium and may or may not be characterized by the same dielectric constant. We will be studying the properties of carriers in thermal equilibrium.

The dielectric constant of semiconductors at microwave frequencies is usually studied in guided structures whereas at optical frequencies these studies are conducted in free space. In the millimeter wave region one could, in principle, take either approach. We have been able to obtain more reliable results by free space measurements which we will describe below. Our measurements were performed on n-type single crystal silicon at a frequency of 107 GHz.

We measured the reflectance, R, and transmittance, T, of a silicon wafer of uniform thickness for plane wave incidence. The solution of R and T as a function of the relative permittivity of the medium,  $\kappa=\kappa'$ -j $\kappa''$ , the thickness, t, of the wafer and the polarization of the incident radiation is well known. We determined the relative permittivity from a measurement of R, T and t using the system shown in Figure 1. The millimeter wave source, manufactured by Varian, emits radiation at 107.3 GHz. To determine the reflectance, R, we measured the signal at receiving horn 2 with the silicon wafer in place and with the silicon wafer replaced by an aluminum slab. Assuming the aluminum slab behaved as a perfect mirror, the reflectance of the silicon wafer could be determined as the ratio of the two measurements. The transmittance was determined as the ratio of the signal received at horn 1 with the silicon wafer in place and the silicon wafer removed.

When the silicon wafer is positioned so that its surface is perpendicular to the direction of propagation of the incident radiation, resonances between the horns and the wafer can occur. These interactions have the form of a residual standing wave pattern such that the received millimeter wave signal is a sinusoidal function of position with a period of  $\lambda/2$  (where  $\lambda$  is the free space wavelength). The standing waves were practically eliminated by rotating the silicon wafer so that the surface normal is at an angle,  $\theta$ , with the direction of incidence.

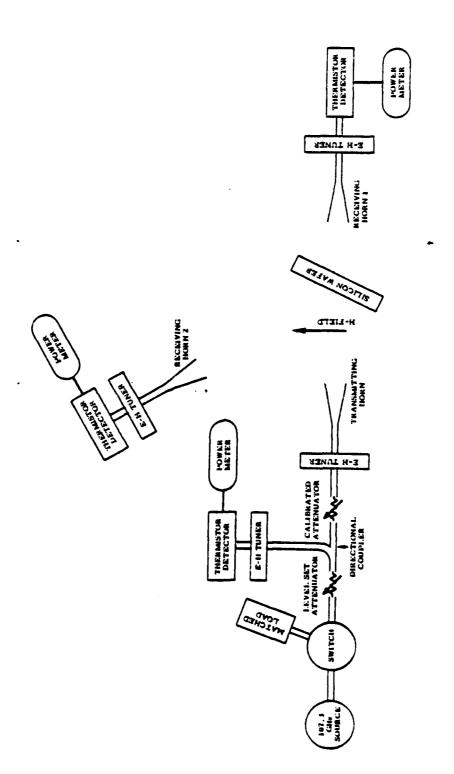


Fig. 1. Millimeter wave measurement system.

In our experiment we used an angle  $\theta$  of about 17 degrees. Although residual standing wave interactions can still occur, they are minor, and the measurement is performed by averaging the received signals with the receiving horn at two longitudinal positions spaced  $\lambda/4$  apart. 2,3

Another experimental problem that we encountered was a deviation from plane wave conditions due to radiation from the edges of the wafer and wafer holder. This deviation gave rise to a transverse interference pattern. This effect was greatly reduced by using a tapered millimeter wave absorber to cover the edges of the wafer and wafer holder.

Our measurements were performed over two resistivity ranges. Both transmittance and reflectance measurements were obtained in the 5-46 ohm-cm range whereas in the 0.007-5 ohm-cm range only reflectance measurements could be obtained because the wafers became too absorbant to obtain reliable transmission data. In Figure 2 the points represent the values of  $\kappa^\prime$  and  $\kappa^\prime$  determined from our experimental measurements of reflectance and transmittance. In Figure 3 the points represent our measured reflectance.

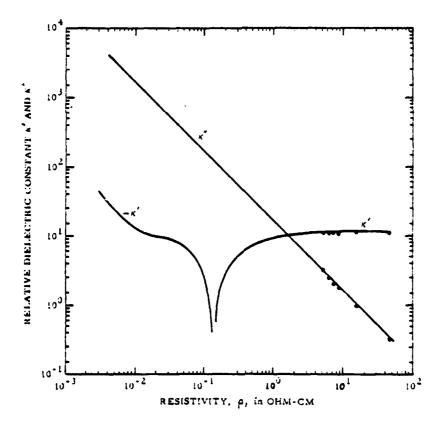


Fig. 2 The real and imaginary parts,  $\kappa'$  and  $\kappa''$ , of the relative permittivity as a function of resistivity  $\rho$ . The points are measured and the solid line is the theoretical prediction based on the Drude model.

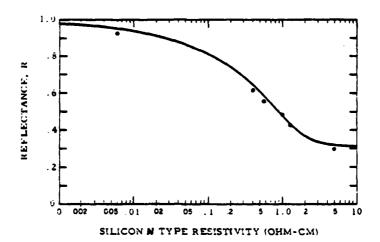


Fig. 3 The reflectance R as a function of resistivity  $\rho$ . The points are measured, and the solid line is the theoretical prediction based on the Drude model.

Our experimental data in these two graphs are compared with the theoretical predictions of a simple Drude model with an energy-independent collision frequency,  $\upsilon$ . For an applied electric field, varying harmonically as  $\exp(j\omega t)$ , we treat the electron as a classical point charge subject to collisional damping and write the relative permittivity,  $\kappa$ , of silicon as a sum of a wavelength independent contribution of the intrinsic crystal,  $\kappa_{\infty}$ , and a varying contribution of free carriers arising from impurities,

$$\kappa = \kappa_{\rm p} - (\omega_{\rm p}^2/\omega^2) (1 - j \frac{\upsilon}{\omega})^{-1}$$
 (1)

where  $w_p^2 = Ne^2/m^*\epsilon_0$ , N is the donor impurity concentration, e is the electronic charge,  $m^*$  is the electron effective mass and  $\epsilon_0$  is the vacuum permittivity. The above model also yields the expression for resistivity

$$\rho^{-1} = \omega_{\mathbf{p}}^2 \ \epsilon_0 \ \upsilon^{-1} \tag{2}$$

To determine  $\kappa$  we first measured the resistivity,  $\rho$ , of the silicon wafer using a colinear four point probe. The impurity concentration, N, is determined from National Bureau of Standards data (N is a function of  $\rho$ ). The collision frequency,  $\upsilon$ , can then be determined from (2) above and the results substituted in (1) to determine the relative permittivity,  $\kappa$ , as a function of resistivity as shown in Figure 2. From these values we can also compute the reflectance, R, as a function of resistivity as shown in Figure 3.

The high resistivity data shown in Figure 2 indicates that the experimentally determined values of  $\kappa'$  and  $\kappa''$  are in good agreement

with the predictions of the Drude model. Our lower resistivity data in Figure 3 indicates that our measured reflectivity is also in good agreement with the Drude model. This result was also found in the infrared region<sup>5</sup> over a frequency range of  $200-1000 \text{ cm}^{-1}$  (1 cm<sup>-1</sup> = 30 GHz).

On the basis of the above data we conclude that we can use a simple Drude model to predict the dielectric constant of n-type silicon over a wide resistivity range at a wavelength of 3mm.

#### 4. REFERENCES

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- 3. W.E. Vaughan, W.S. Lovell, and C.P. Smyth, J. Chem. Phys. 36, p. 535 (1962).
- 4. B. Senitzky and S.P. Weeks, J. Appl. Phys., 52, p. 5308 (1981).
- 5. ASTM F723-81, Standard Practice for Conversion Between Resistivity and Dopant Density for Boron Doped and Phosphorous Doped Silicon.

#### 5. Dod and other interactions

Measurements on silicon similar to the ones described here, but in the far infrared region (2-50  $\mu m)$ , were made in collaboration with S.P. Weeks of the Bell Telephone Laboratories. Their interest was in developing a reliable technique for thin epitaxial silicon layers.

# C. ACOUSTOELECTRIC AND ACOUSTOOPTIC DEVICES

Professors W.C. Wang and H. Schachter

Unit SS2-3

# OBJECTIVE(S)

The objectives are:

- (a) To study the physical phenomena underlying the performance of surface acoustic wave devices employing nonlinear effects in semiconductors, and in the process to improve device performance or invent new devices.
- (b) To examine a new method for diagnosing the surface and interfacial conditions of a thin-film semiconductor by acoustoelectric means.
- (c) To study thin film deposition processes and to develop ZnO and InSb thin films of high quality for acoustoelectric and acoustooptic applications.

# 2. APPROACH

- (a) As part of the study of physical phenomena underlying the performance of SAW devices, a new type of FM demodulator has been developed based on the strong space charge nonlinearity induced by SAW's in an adjacent semiconductor and on the filtering action generated by spatial integration over the length of the nonlinear interaction. This type of FM demodulator is structurally very simple and can be operated at high carrier frequencies; its performance is presently under study.
- (b) A theory based on the nonlinear interaction between induced charges and fields has been developed in order to describe the operation of a semiconductor thin-film convolver at flat band. In the past, various convolver theories have been proposed and presented, but those theories were valid only for semiconductors of thickness large in comparison with the acoustic wavelength. One of the reasons for developing such a thin-film theory is that it will help in the diagnoses of thin-film surfaces and interfacial properties. Using SAW as a diagnostic tool, the advantages are (i) the depth of electric field penetration can be controlled by varying the sonic frequency; thus, the interfacial properties of the thin film can be investigated, (ii) the diagnostic process is contactless and nondestructive, and (iii) the electric field associated with the SAW's has both tangential and normal components, so that some of the thin-film orientational properties can be revealed. Computer results for thin-film convolvers at flat band have been obtained. Theories and models for the non-flat band case will be devel-The results will be used to evaluate the experimental outcomes.

(c) We are developing a new method for depositing ZnO films of high quality using a specially-modified sputter S-gun system. Using this new method, a systematic study will be made of such films deposited on various substrates at various temperature levels to optimize the technique and the conditions of operation. We are also studying techniques for improving the deposition of InSb films and avoiding a layer of Sb-InSb-In. In this connection, we are examining a flash evaporation scheme with a special preheating procedure.

# 3. PROGRESS

During the contract period we have made the following major accomplishments.

- (a) We have successfully designed and constructed a novel and superior thin film deposition system utilizing a modified sputter gun. This new system permits us to fabricate thin piezoelectric or semiconducting films of exceptionally high quality at both low temperature and low pressure. The new system has many additional advantages: it is cost effective (low cost both to construct and to operate), it has a high deposition rate (comparable to that of the more costly and less advantageous planar magnetron system), it reduces greatly the problem of thermal stresses, and it permits the fabrication of clear, well-oriented, high quality films on many different substrates, in contrast to other systems.
- (b) Using our newly-developed sputtering system, we have fabricated excellent thin films of ZnO and AlN on various substrates. Good InSb films have also been made using evaporation techniques. The ZnO films, which came first, are as good as any made elsewhere, to our knowledge, and have received high praise from industry. We have also fabricated them on glass, silicon and quartz substrates, with equal facility and quality. The low pressure associated with our sputtering system permits us to produce AlN films of exceptional quality, colorless and with an extremely smooth surface. The InSb films we have produced are not yet of top quality, but to our knowledge they are the best in the world outside of the Soviet Union, and we have achieved bidirectional SAW amplification with them, which indicates that they are already quite good.
- (c) Because of discrepancies which consistently appeared in experimental data involving the acoustoelectric (AE) effect, we theoretically examined the Weinreich relation, which relates the acoustoelectric current to the acoustic power loss and the carrier mobility. A two-dimensional analysis was carried out on a configuration consisting of a semiconductor film on a SAW substrate, taking into account both the transverse and tangential dc acoustoelectric effects. It was found that the Weinreich relation, which is widely used and assumed to be correct, is not valid most of the time it is used in SAW configurations. Its range of validity is difficult to express simply, but we are currently clarifying it.

(d) Since monolithic thin film semiconductor convolvers are of substantial interest and should become feasible now that very good thin films can be fabricated, we examined the properties of several possible types of such convolvers. The stress in the study was on the semiconductor film on a piezoelectric substrate, which should have a time-bandwidth product comparable to that of the successful but inconvenient separated-medium type. We made calculations on the dispersion, attenuation, and efficiency, as a function of film thickness, conductivity and frequency, for two types of output terminal arrangement. These analyses involved new considerations, not taken into account by available theories.

These accomplishments have led to a series of publications and talks, the most recent of which are presented in Section 4.

Some of the details regarding our progress and accomplishments are briefly summarized below.

# A. ZnO Films Grown at Low Temperature by Our Newly Developed "Modified Sputter Gun" System

The deposition of C-axis oriented ZnO films by a sputtering technique was initiated in the mid-1960s. Since then, ZnO films have been considered to be one of the most promising materials for optical waveguiding, acoustoelectric applications, acoustooptic interaction media, and SAW transducers, based on its high electromechanical coupling coefficient and its superior optical qualities. However, ZnO film did not gain momentum until the group at Kyoto University, Japan, reported several years ago that high quality ZnO films can be obtained on 7059 glass substrates at a relatively high growth rate ( $\cong$  2µm/hr) by utilizing planar magnetron sputtering. (The thermal expansion coefficients of ZnO and 7059 glass are nearly identical.) It is of interest that Dr. S. Onishi, one of the collaborators on this work unit, was a key member of that group under Professor Shiosaki, and that the work on planar magnetron sputtering was the topic of his doctoral dissertation.

However, the films on other substrates, such as silicon, quartz, etc., are normally not optically transparent due to their mismatch in thermal expansion coefficients. In order to improve the quality of ZnO films on all substrates, we studied these past techniques and recognized that in order to achieve clear films one must essentially avoid the problem of thermal stress caused by electron bombardment. We then found how to avoid such stress by suitably modifying the "research S-gun" sputtering system. Presently, this modified S-gun provides us with films of the highest quality. The reason why will become clear as we review the past sputtering methods.

(1) Using a conventional sputtering unit: the substrate holder is of positive polarity. While the ionized A ions strike the targets (ZnO or Zn) to remove material for deposition, the electrons are bombarding the substrate since it is at positive potential. As a result, the substrate temperature is arbitrarily high and can not be controlled. Films thus obtained are of poor quality.

(2) Utilizing a planar magnetron sputtering system: With this system, the majority of the electrons are trapped in the magnetic field. Nevertheless, the substrate will still be bombarded by some of the electrons, since the substrate holder is at positive potential. As stated earlier, the planar magnetron system has significantly improved the film deposition technique. However, ZnO films which are well oriented, clear and of high quality are usually difficult to obtain on other than the 7059 glass substrate.

With the so-called "research S-gun" sputtering system, it was necessary for us to augment and specially arrange the magnetic field so that the thin-film surface is completely outside of the plasma column and free from electron bombardment. When these modifications have been made, the S-gun system is the system that has provided us with the best quality of film on various substrates, for the following reasons:

- (a) The substrate holder is at <u>neutral</u> potential, and the substrate surface is free from electron bombardment.
- (b) The water cooling system is very effective, since it is right next to the target. The target will therefore be at a lower temperature and the substrate surface will not be subjected to excessive heat radiation from the target.
- (c) The magnetic field is several times stronger than that associated with a planar magnetron. The plasma column is therefore more tightly confined.
- (d) The deposition rate of an S-gun system is comparable to that of a planar magnetron, whose deposition rate is good.

Therefore, the substrate holder is at a low temperature, around 150°C, rather than about 500°C as with the planar magnetron. This feature is of key significance, since it greatly reduces the problem of thermal stresses. As a result, with this system, we are able to obtain clear, well-oriented, high quality ZnO films on all substrates available to us, such as glass, silicon and quartz substrates.

In addition to the key features of low pressure and low temperature sputtering, other advantages of this newly-developed sputter gun system include: (a) a much larger area of high quality thin film can be obtained, and (b) the system is cheaper to construct and cheaper to run.

# B. Aln Films Grown at Low Pressure and Low Temperature, Utilizing Our "Modified Sputter Gun" System

The utilization of our modified sputter gun has also been extended for the deposition of aluminum nitride (A1N) films on various substrates. The strong magnetic field associated with this gun system makes it possible to maintain a stable plasma at a total sputtering gas pressure (TSGP) as low as 1  $\mu$ Torr. This low-pressure sputtering pro-

vides films with denser and finer grains and it improves c-orientation, surface smoothness, film color, transparency and deposition rate. Our experience shows that the qualities of A1N films are extremely sensitive to the level of total sputtering gas pressure, the lower the better. The total pressure in our system varies from 1  $\mu Torr$  to 8  $\mu Torr$ . The deposition rate of the sputter gun is three times as high as that of a conventional planar magnetron, since the target cooling system makes it possible to increase rf or dc power. It is 2.4  $\mu m/hr$ . at an input power of 300 watts. The film is transparent and colorless only at low pressure sputtering. High quality films are deposited at temperatures around 350°C, which is low for A1N deposition. The substrate surface in this system, as stated in A, is free from charged particle bombardment and excessive heat radiation.

#### C. InSb Films

The deposition of InSb thin films on LiNbO3 substrates has been accomplished at different centers since the early 1970s, and the process has been used with little variation in Japan, France, Russia and the However, due to difficulties in obtaining high quality films, acoustoelectric devices using InSb films have not been proven to be practical. For AE applications it is required that the InSb film possesses high drift mobility and high resistance. The best data reported to date are by Kotelyanskii, et al, in Russia; they can obtain a film of 500A thickness and a drift mobility of 1600 cm<sup>2</sup>/v-sec. This mobility is over three times better than what has been reported in the western world. We have been engaging in the development of InSb films for three years and have achieved bidirectional SAW amplification with those films (necessary for reducing the insertion loss of a convolver). drift mobility we obtained here is  $\cong$  700 cm<sup>2</sup>/v-sec at a film thickness ~ 500A, which is better than what is reported in this country but is still low in comparison with that of Kotelyanskii, et al. Private discussions with Kotelyanskii during his recent visit to us here revealed that their set-up is much more elaborate and costly, and they have invested 10 years in this effort.

We have measured the Hall mobility as a function of the conductivity thickness product. The film thickness is about 450Å. Our process, especially on forming the electric contacts, we feel is superior. The highest Hall mobility obtained by us is about 2500 cm/volt-sec, which means that if the traps can be eliminated in this film a drift mobility of that same magnitude can be achieved. The significance of these measurements is that they tell us how good a film can be achieved ultimately, when the Hall and drift mobilities are equal. Thus, these measurements offer us substantial hope.

# D. Examining the dc Acoustoelectric Current Produced by SAW

It is generally believed that surface acoustic waves will be useful in determining the surface and interfacial properties of semiconductor wafers and semiconductor films; however, in the process of our correlating data from SAW measurements with those obtained from conventional methods, some discrepancies consistently appear. This led us to

examine the validity of the commonly-used <u>Weinreich relationship</u> for a configuration consisting of a semiconductor on a SAW substrate. The Weinreich formula relates the acoustoelectric current to the acoustic power loss and the carrier mobility. Since both the AE current and the power loss are measurable quantities, the carrier mobility can thus be determined. Comparing the mobility measured here with the Hall mobility measurement, trapping dynamics can also be revealed.

The Weinreich relation was first derived for phonon-drag phenomena in Ge due to the deformation potential. Its validity in bulk piezoelectric semiconductors and in the presence of acoustic gain was experimentally verified by one of us (W.C. Wang) in 1962, and subsequently analyzed by H.N. Spector. In examining the Weinreich formula for thin films, however, we have carried out a two-dimensional analysis for a configuration consisting of a semiconductor film on a SAW substrate, taking into account both the transverse and tangential dc AE effects. The analysis shows that the range of validity of the Weinreich relation in such a system is very limited and that in general it cannot be applied here. (Its range of validity cannot be simply stated, but we are currently assessing the validity conditions.) In addition, the analysis reveals that (a) the field associated with the transverse AE current in general tends to accumulate the charge at the semiconductor surface, (b) the polarity of the transverse AE current will, in general, not change sign when the film thickness is larger than the SAW wavelength, and (c) the diffusion effect cannot be ignored in the calculation of tangential AE current.

# E. Monolithic Thin Film Semiconductor Convolver

Many forms of convolver have been designed and tested. The best performance to date is the one given by the <u>separated-medium</u> Si on LiNbO<sub>3</sub> normal-component convolver fabricated at Lincoln Laboratory and Texas Instruments. However, looking ahead and taking into consideration eventual cost effectiveness and smaller size, the monolithic convolver still remains a strong candidate. There are three possible monolithic AE convolver structures: (i) piezoelectric film on semiconductor substrate; (ii) semiconductor film on piezoelectric substrate; (iii) piezoelectric film on semiconductor film. The time bandwidth (TB) product for case (i) is usually rather low due to the dispersion introduced by the piezoelectric film (operating in the Sezawa mode). The TB product for case (ii) should be comparable to that of the separated medium type. Therefore, we started to analyze its performance. Case (iii) will be investigated in the future.

Two types of output terminal arrangement for case (ii) have been investigated. In one type, the output terminal plate is in direct ohmic contact with the top of the semiconductor surface, and in the other an insulating dielectric layer is inserted between the semiconductor surface and the convolver on the output plate. Therefore, the former has a short-circuit condition and the latter an open-circuit condition on the semiconductor surface. Since the boundary conditions are different, the velocity, attenuation constant and convolver efficiency are found to be quite different in the two configurations. Calculations on the dis-

persion, attenuation and efficiency have been carried out as a function of film thickness, conductivity and frequency.

During the past year we have been engaged in the development of an active thin film monolithic convolver. We have had some success in experimental work and theory for the structure comprised of InSb on  $LiNbO_3$ .

Two convolver configurations were investigated. One utilizes the transverse field component (width direction) induced by the SAW, and the other uses the tangential component. The operational principle of the transverse convolver is still not clear and its investigation is continuing. In the discussion below, the device based on the tangential field component is described only briefly. On the other hand, the work on the transverse convolver, which has recently been found to be more efficient, is treated in some detail.

# (1) An Active Transverse Mode Thin Film InSb/LiNbO3 Convolver.

Introduction: An integrated and combined thin film InSb on LiNbO<sub>3</sub> convolver and amplifier device was constructed. The device was operated successfully at 150 MHz with an insertion loss around 6 dB. The convolver output, which was taken in the width direction, transverse to both the sonic propagation and the substrate normal, was greatly enhanced by the application of a transverse (width direction) drift d.c. field on the InSb film. Since the width of InSb film can be made narrow, the d.c. voltage required is not excessive. The relationship between the convolver output and the transverse d.c. field is approximately linear. Understanding of the operation of such a configuration is still not clear. Theoretical analysis is presently in progress. In the near future, this type of output enhancement is to be extended to other thin film structures such as ZnO or Si.

Fabrication Process: Indium antimonide on LiNbO<sub>3</sub> is one of the best combinations for use in a surface acoustic wave amplifier (SAW AMP)<sup>7-9</sup> as well as for a convolver. <sup>10,11</sup> High mobility InSb films are very difficult to obtain because of the difference in vapor pressure between In and Sb. The InSb tends to fractionate, resulting in a layered film structure consisting of Sb, InSb, then In. A simplified flash system was built to get more consistent, homogeneous InSb films and thus higher mobility InSb. Cominco Grade 69S is crushed to fine particles, placed on a belt conveyer and dropped via a chute into a V-shaped, resistance-heated molybdenum boat. The substrates consist of a barrier layer of 900 Å thick SiO deposited on Y-cut, Z-propagation LiNbO<sub>3</sub>. A quartz crystal oscillator is used to monitor the 400-700 Å thick InSb films during deposition on the substrate, which is at 300°C.

The high mobilities for thin films of InSb are obtained only after annealing at a temperature near their recrystallization point. At this temperature, the thin (400-700 Å) InSb film required for a SAW AMP loses a significant amount of material through re-evaporation. A thin cover film of an inert dielectric material deposited over the InSb will

minimize this problem; however, good contacts become hard to achieve. Conventional dielectric materials, such as SiO,, SiO2 or Al2O3 cannot be etched off after annealing because the required acid also etches off the InSb film. These materials therefore make it necessary to deposit the contact film prior to deposition of the protective film and to anneal-At the recrystallization temperature, the deposited contact material tends to diffuse into or alloy with the InSb film, adversely affecting its electric properties. An AlN cover film solved these problems. AlN is easily etched with an alkaline solution which is harmless to InSb. This allows contact to be made with the film after annealing by using photolithography techniques to etch "windows" in the A1N and then depositing aluminum contacts. 12 The whole surface is covered with 800 A of A1N by reactive sputtering<sup>2</sup> after which the film sandwich is annealed at temperatures between 519-623°C. After etching out "windows" in the AlN, 1000 A thick Al contacts are deposited on the three InSb films, while the interdigital transducers (IDT) are deposited on LiNbO<sub>3</sub> during the same deposition.

Experimental Results: The active convolver consists of three InSb thin film sections. Drift pulses are applied to the two end InSb films providing SAW amplification. Convolution processes are performed at the center InSb film. Convolution signals are greatly enhanced by applying d.c. pulses to the center film in the direction transverse to both the sonic propagation and the substrate normal. The conventional normal component convolver usually suffers from the capacitance coupling caused by LiNbO3 substrate. The newly designed convolver eliminates this capacitive coupling by picking up the signal directly from the center semiconductor film. This film does not function as a SAW AMP, but provides a high S/N ratio and a high efficiency convolution signal with bias pulse. The design parameters of the interdigital transducers are as follows: finger pair 12; wavelength 23.2 µm; and aperture 1.0 mm. The operational parameters are shown in Table 1.

TABLE 1. The Operational Parameters of Integrated InSb Convolver

DRIFT PULSE	BIAS PULSE	INPUT RF PULSE	CONVOLUTION OUTPUT SIGNAL	EFFICIENCY OUTPUT INPUT
-800V (1.6kV/cm)	±200V	3.85Vpp 1µ	s 0.49Vpp	-17.9dB
0V	±200V	3.85Vpp 1µ	s 0.02Vpp	-45.6dB
-800V (1.6kV/cm)		3.85Vpp 2µ	*	-6±1.7dB

<sup>\*</sup> Tangential component convolver with pre-amplifier and reference signal.

The bias pulse can be of either plus or minus voltage, resulting in the same output. An input-output efficiency of -17.9dB has been achieved with this device. This output convolution signal provides enough power to eliminate the preamplifier or mixer reference signal. These performances are from preliminary experimentation and do not represent optimization for highest efficiency convolvers. Properly optimized design will be needed before the full potential of this structure can be established.

# (2) Active Tangential Mode Thin Film InSb/LiNbO<sub>3</sub> Convolver.

A detailed theoretical analysis has been carried out for the tangential mode thin film convolver. In the convolver operation both the forward and backward waves are amplified, i.e., the SAW amplifier is bi-directional. The same InSb film strip is used for amplification and convolution in the device geometry. Calculations on the convolver efficiency as a function of drift field, film thickness and conductivity have been made. Since the geometry of the multi-layer structure, InSb on LiNbO<sub>3</sub> with a very thin passivation layer of SiO<sub>2</sub> sandwiched inbetween, is very similar to that of a separated medium amplifier and convolver, the techniques used in the analysis is quite similar to that for a separated medium one. However, it is much more involved here since bi-directional gain has to be considered. Experimentation on the bi-directional tangential mode active convolver was also carried out; the convolver efficiency has been found to be far less than that of the transverse mode convolver described in the previous section.

#### 5. PUBLICATIONS

- 1. "Transparent and Highly Oriented ZnO Films Grown at Low Temperature by Sputtering with a Modified Sputter Gun," by S. Onishi, M. Eschwei and W.C. Wang, Applied Phys. Lett., vol. 38(6), p. 319 (1981).
- 2. "Colorless-Transparent, c-Oriented Aluminum Nitride Films Grown at Low Temperature by a Modified Sputter Gun," by S. Onishi, M. Eschwei, S. Bielaczy, and W.C. Wang, October 15, 1981 issue of Applied Phys. Lett.
- 3. "Properties of InSb Film for SAW Amplifier," by M. Eschwei, S. Onishi and W.C. Wang, American Vacuum Society 28th National Vacuum Symposium (1981).
- "Monolithic Thin Film Acoustoelectric Convolver," by Z.S. Wu, S. Onishi, K.S. Chen and W.C. Wang, 1981 Ultrasonics Symposium.
- 5. "Acoustic, Optical Properties of A1N Films Grown at Low Temperature by Modified Sputter Gun," by S. Onishi, M. Eschwei, S. Bielaczy and W.C. Wang, 1981 Ultrasonics Symposium.

- 6. "D-C Acoustoelectric Current Induced in a Semiconductor Film Adjacent to a SAW Substrate," by K.S. Chen, Z.S. Wu, H. Schachter and W.C. Wang, 1981 Ultrasonics Symposium.
- 7. G.S. Kino, T.M. Reeder, IEEE Transaction on Electron Devices, <u>ED-18</u>, 909 (1971)
- 8. I.M. Kotelyanskii, A.I. Krikunov, A.V. Medved, R.A. Mishkinis and V.V. Panteleev, Sov. Phys. Semicond., 12, 751 (1978).
- 9. Yu. V. Gulyaev, I.M. Kotelyansky, A.V. Medved and R.A. Mishkinis, Electronics Letters, <u>16</u>, 115 (1980).
- 10. L.A. Coldren and G.S. Kino, Appl. Phys. Lett. 23, 117 (1973).
- 11. K. Yamanouchi, S. Mitsui and K. Shibayama, IEEE International Microwave Symposium, p. 31 (1980).
- 12. M. Eschwei, S. Onishi, F. Cassara and W-C. Wang, J. Vac. Sci. Technol., 20, 873 (1982).

#### 6. Dod and other interactions

Industry has expressed substantial interest in our thin film fabrication capability and its potential for producing excellent films in a cost-effective manner. Three examples are given:

- (a) Fairchild Camera and Instrument is discussing with us a program which would utilize an InSb thin film amplifier in the construction of a compact and low loss SAW delay line for repeater-jammer applications. Negotiations with Mr. E. Magill are in progress.
- (b) Hazeltine Corporation is discussing with us a program to develop ZnO thin films on quartz for wideband transducers. Negotiations with Dr. R. LaRosa are in progress.
- (c) The earliest public recognition of our capability was made by Dr. F. Hickernell of Motorola, Arizona, with whom we were in contact. During his invited talk on ZnO thin films at the 1979 IEEE Ultrasonics Symposium, he held up one of our high quality (transparent and colorless) ZnO films on glass and stated that this is an example of what a really good film should be like.

In addition, we have had visits and arrangements to visit us from a large variety of sources. Some examples are:

(d) Drs. J.M. Kotelyanskii and V.T. Potapov of the Institute of Radioengineering and Electronics, Academy of Sciences of the USSR, Moscow, visited us in Brooklyn (and therefore did not see our facility, which is in Farmingdale), and we exchanged information on InSb films. Dr. Kotelyanskii's laboratory produces the best InSb films in the world.

It is of interest that about one month later, at an URSI General Assembly in Washington, DC, Professor Oliver was approached by a "young scientist" delegate, Dr. V.I. Anisimkin, from the same laboratory in the USSR, who referred to that meeting and asked if he could spend up to six months in Professor Wang's laboratory.

- (e) Professors P. Kornreich and S. Kowel of Syracuse University visited us to discuss our AlN and ZnO deposition techniques.
- (f) Dr. H. Gautier and Dr. P. Defranould of Thomson-CSF, Cagnes sur Mer, France, visited us just after the 1981 IEEE Ultrasonics Symposium.
- (g) Among others who have visited our facility are Mr. E. Stern of the MIT Lincoln Laboratory and Professor P. Das of the Rensselaer Polytechhnic Institute.

# D. ELECTRIC AND MAGNETIC INTERACTIONS IN THIN FILMS AND SURFACE REGIONS OF SOLIDS

Professor H.J. Juretschke

Unit SS2-4

# 1. OBJECTIVE(S)

To understand the equilibrium properties, the approach to equilibrium, and the response to applied fields and waves of the surface regions of selected solids, both conductors and insulators, and to develop new methods for their investigation.

#### APPROACH

The experimental approach concentrates on the change of properties of solids when the surface/volume ratio of their geometry becomes significant. Transport properties are examined for their size effects, and on the influence of specific parameters, such as electrostatic charging, changes of composition or of order, or mechanically induced surface strains, on these size effects. Emphasis is on those special interactions that lead to nonlinear responses or to resonances, and on the coupling between the electromagnetic and elastic fields in the surface region. The theory will emphasize use of the methods developed in recent years for the study of defects in solids for the investigation of the surface, considered as an extended defect.

#### 3. PROGRESS

The main emphasis during the report period has been in the two areas:

- A. Charge-induced surface stresses at metal surfaces
- 3. Surface layer self-diffusion.

Except for item (1), below, our progress will be summarized separately for areas A and B.

(1) Work in both areas has been backed by the development of a new theoretical model of conduction-electron surface scattering, that is based on scattering in depth within a surface layer of electrical properties differing from those of the underlying material. This theory, incorporating effects of thermal surface phonons as well as of geometrical rearrangements, has been submitted for publication. Its predictions both overlap and differ from those of other treatments of surface scattering. Thus, as expected, surface scattering becomes more important as either the sample thickness decreases, or the carrier mean free path increases, but the universal behavior in terms of the ratio of these two lengths characteristic of most other models is no longer true. In addition, surface phonons may predict spurious asymptotic values, and temperature-independent surface structures may simulate temperature-dependent surface scattering, if interpreted in terms of those models.

# A. Charge-induced Surface Scattering

- (2) The effect of surface charging on electron scattering at well-annealed metal-vacuum interfaces has now been measured extensively on samples of Ag, Au, and Cu, in the range  $1.8 \le T \le 300^{\circ} \text{K}$ . The data, though individually ranging over factors larger than 100, are interpreted successfully in terms of the nearly universal scaled behavior predicted by our theory, for values of the scaling parameter K (= sample thickness/bulk mean free path) ranging over as much as  $10^3$ . The temperature-independent surface charge density dependence of the surface strain is about  $0.1/(\text{C/m}^2)$ , for Ag.
- (3) The mean penetration depth of surface strains at these well-annealed surfaces has been determined to be about 10 to 15 Å, Charged-induced scattering, which alters this depth by a very small amount ( $\sim 10^{-5}$ ) can be suppressed if the metal surface is covered by a layer of graphite of this order of thickness. Graphite has been found to present less problems as a very thin layer than the previously attempted gold.
- (4) For both Ag and Au, positive charging increases the surface strain, in accord with the increase in perpendicular lattice constant observed on most metal surfaces. The opposite sign, seen in Cu, has been found to arise from the rapid oxidation of any exposed copper surface, and reflects the influence of adsorbed gases on surface strains.
- (5) The strains induced in all samples by Maxwell stresses (i.e., proportional to  $q^2$ , where q is the surface charge per unit area) also produce changes in (volume) scattering, in the same range of temperatures for which we have studied surface strain scattering. This volume scattering shows first an anomalously large increase as the temperature is lowered, and is then followed by a precipitous drop, often to complete vanishing, at temperatures below about 7°K. Both aspects of this behavior are unexpected and, so far, unexplained. One obstacle to understanding this is the complete absence of experimental or theoretical information on the strain sensitivity of the bulk conductivity of metals at low temperatures. Another is the uncertainty in the stress distribution and therefore the strain distribution caused by finite sample size, which is very sensitive to sample geometry. An additional possibility that remains to be explored is that surface strains also contain a contribution quadratic in q at very low temperatures.
- (6) Charge-modulated surface scattering at the Ag-Mica interface follows roughly the same behavior as at the free surface, for  $T \geq 60^{\circ} K$ . However, new results below this temperature show that surface strain scattering reverses sign, and is accompanied by a contribution quadratic in q peaked at the cross-over, but of opposite sign to that induced by Maxwell stresses. A similar effect had been seen earlier in Au, but, occurring at a much higher temperature, it is far less dramatic and far less detailed. The low temperature data for the Ag-Mica interface indicate that this interface is much more complex than

the free surface, and that it probably includes interfacial strains arising from a temperature-dependent epitaxial mismatch of the two adjacent materials. If properly interpreted, the data should become a rich source of information on such interfacial strains.

# B. Disorder-induced Surface Scattering

- (7) Experiments on the initial response of surface scattering to a disordered Ag overlay deposited on a flat silver surface at low temperature show that surface scattering saturates when the layer thickness exceeds about 20 Å, indicating that above that thickness the overlay acts like a perfect absorber of incident electrons. Consequently, the use of surface scattering to investigate the layer structure is most sensitive for smaller layer thicknesses.
- (8) For each surface layer structure, we have found a temperature  $T_{\rm c}$  below which surface scattering is fully reversible as the temperature T moves up or down. But once T exceeds  $T_{\rm c}$ , surface scattering decreases irreversibly, first very fast, and then more slowly. By proper choice of the excess temperature and the time interval during which it is maintained before the temperature is reduced again, a new reversible temperature range for surface scattering, and a new  $T_{\rm c}$  for this next stage of annealing, can be established. These characteristics follow very much those of a typical glass-crystalline transition.
- (9) By dividing this process of partial annealing into about ten stages, and then analyzing the reversible region below each  $T_{\rm C}$  in terms of our theory (item 1, above), we have been able to interpret the scattering data in terms of an effective disturbed layer thickness and an effective disorder parameter within that layer, as a function of  $T_{\rm C}$ . The first results of such analysis show that the layer thickness first reduces slowly and then more rapidly, and stabilizes at between 10 and 15 Å, and that the disorder parameter first decreases rapidly, and then more slowly as annealing proceeds, and also stabilizes at a finite value. Both trends are in good agreement with the numbers obtained, in a completely different experimental manner, under item 3 above. However, other implications of the theory have to be confirmed before this interpretation can be fully accepted.
- (10) We have been able to establish satisfactory experimental conditions for following the change of surface scattering as a function of time at a given T, and are thus able to determine the effective activation energies connecting any two stages of annealing. As expected, the activation energy increases as the annealing approaches completion.
- (11) In the final stages of annealing,  $T_{\rm C}$  increases rapidly, though still staying well below room temperature, indicating that there is an extended tail of high activation energies that have to be overcome

before the surface is stable and reversible under changes of temperature. We hope to be able to establish by a more detailed study whether these high energy sites belong to the outer surface, or to the overlay-base interface.

Items 2 to 6 represent work contained in a Ph.D. thesis to be completed by June 1982.\* Its results will appear in a number of papers. Items 7 to 11 are part of another Ph.D. thesis currently in progress.\*\*

#### 4. PUBLICATIONS

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- 2. H.J. Juretschke and R. Pimpinella, "Size Effects in Thin Metallic Films Resulting from Modified Surface Transport Properties," submitted to Surface Science.
- 3. R. Pimpinella and H.J. Juretschke, "Low Temperature Anomalies in the Surface Charge Modulation of Thin Metallic Film Conductance," to be published.
- 4. R. Pimpinella and H.J. Juretschke, "Thin Film Surface Structure Determined by Surface Scattering of Conduction Electrons," to be published.
- 5. Y. Amani and H.J. Juretschke, "Transport in Thin Films with Rough Overlays," to be published.

#### 5. Dod and other interactions

In view of our extensive experience with the physics of strains on metal surfaces, gained largely under JSEP support on this work unit and its predecessor, we were asked by AFOSR about three or four years ago to advise it on the RADAM problem, involving the modulation of radar scattering by moving or vibrating contacts. This consultation led to a separate contract with AFOSR to determine the effects due to the intrinsic nonlinear electrical properties of weathered and rusty metal surfaces. In particular, we investigated the role of microscopic metal-oxide barriers. We found that they allow tunneling of electrons through surprisingly thick barriers, and at low energies, and that the sensitivity of such barriers to macroscopic strain is large, but not quite large enough to explain the modulation effects on that basis alone.

<sup>\*</sup> R. Pimpinella, "The Metallic Field Effect and its Relation to Structural Properties of Metal Surfaces."

<sup>\*\*</sup> Y. Amani, "Equilibrium and Non-equilibrium Structures of Silver Surfaces."

# E. NEW SOLID STATE MATERIALS

Professor E. Banks

Unit SS2-5

## 1. OBJECTIVE(S)

To synthesize, characterize and measure the physical properties of new solid state materials. Such materials are potentially ferroelectric (and optically nonlinear), ferromagnetic, fluorescent or semiconducting, all of which have considerable technical interest and value if the properties investigated can be applied to practical devices. Even when they are not of immediate practical value, the study of their properties can lead to understanding that may point the way to the design of improved materials.

#### 2. APPROACH

Attempts to synthesize new materials with interesting electronic properties are based either on modifying existing materials (e.g., by forming solid solutions) or by attempting the synthesis of materials based on theories which attempt to explain the dependence of the relevant property, e.g., ferromagnetism, on features of crystal structure and chemical bonding. New materials are characterized by crystallographic methods and measurement of relevant electronic properties such as optical spectroscopy, fluorescence, magnetic properties, Mössbauer spectra, conductivity and dielectric properties.

#### 3. PROGRESS

# (a) Complex Fluorides of Bivalent Rare Earths: Potential Laserand Scintillation Counters

Experiments on crystal growth of the new compounds, EuMgF4 and SrMgF<sub>4</sub>, failed previously because the compounds melt incongruently, decomposing to the simple fluorides. During the past year, however, we have found that mixtures of SrMgF<sub>4</sub> with BaMgF<sub>4</sub> can be melted without decomposition up to 70 mole % SrMgF<sub>4</sub>. Boules of these mixtures have been found to have a uniform composition. This means that, under suitable conditions, single crystals of such solid solutions should be capable of growth. Polycrystalline boules of 90% BaMgF<sub>4</sub>, 10% EuMgF<sub>4</sub> have been observed to fluoresce bright blue under x-ray excitation. Since the optimum brightness in the SrMgF4-EuMgF4 system occurs at 75% EuMgF4, we can expect more efficient x-ray detection at compositions from 50-74% EuMgF<sub>4</sub> in the BaMgF<sub>4</sub> system. With such a high concentration of heavy elements (Ba, Eu) the x-ray sensitivity should be very high. Crystals of such properties should be very useful detectors for x-rays and other ionizing radiation. They would have the advantage over current crystals, based on CsI, of being resistant to moisture, and even very small crystals would be useful for array devices and medical applications, such as CAT scanners.

An x-ray structure analysis of the three new compounds has been completed, and they are all centrosymmetric -- unlike  $BaMgF_4$ , which is non-centro and hence piezoelectric at room temperature. The solid solutions should have composition-dependent ferroelectric transition temperatures, creating the possibility of preparing compositions whose fluorescence can be modulated by applied electric fields.

The incongruent melting of  $SrMgF_4$  has been confirmed by a determination of the phase diagram of the binary system  $SrF_2$ - $MgF_2$ , using differential thermal analysis (DTA). The system shows an eutectic at 48.4 mole %  $MgF_2$  and 871°C, and a peritectic decomposition at 50 mole %  $MgF_2$  and 880°C, corresponding to  $SrMgF_4$ . A solid-solid transition in  $SrMgF_4$  occurs at 809°C. In spite of the very narrow region of coexistence of  $SrMgF_4$  with the melt (8 degrees in temperature, about 2% in composition) we succeeded in growing  $SrMgF_4$  crystals of about 1 mm size by extremely slow cooling of a stoichiometric melt. Since our previous crystal growth experiments on the  $BaMgF_4$ - $SrMgF_4$  have shown the congruent melting behavior of  $BaMgF_4$  extending to 75%  $SrMgF_4$ , we expect to be successful in growing sigle crystals of these materials.

In the continuation of this program, major emphasis will be placed on the single crystal growth problem, as this is crucial to all experimental work, both of the basic and applied sort. The concentration will be on direct melting and Bridgman crystal growing experiments on the solid solutions of the BaMgF $_4$ -SrMgF $_4$  system, and the BaMgF $_4$ -EuMgF $_4$  system, focusing on the higher (50 mole % and above) concentrations of Sr and Eu compounds.

Initial studies of these crystals will deal with the transition from non-centric to centric crystal symmetry as a function of composition and temperature, followed by studies of ultraviolet-excited fluorescence of the Eu-doped materials over the range from cryogenic temperatures to the temperature of fluorescence quenching (expected to be above room temperature). If the expected ferroelectric phase transitions are detected, studies of the effect of such transitions on the luminescence will be made. Other experimental measurements, such as  $^{19}{\rm F}$  NMR studies,  $^{151}{\rm Eu}$  Mössbauer studies and Eu²+ EPR studies, will be taken to obtain a more detailed understanding of the nature of the transitions and their effect on the local environment of the Eu²+ ion in the crystals.

The expected ferroelectric transitions in the  $BaMgF_4$ -SrMgF\_4 suggests an additional possible application for these materials. There is currently a great interest in solid-state devices for millimeter wave applications, using the dielectric properties of the solid to control the transmission and reflection of the microwaves. At these extremely high frequencies, low-loss, high permittivity materials are required. A ferroelectric material containing ions of low polarizability such as Sr, Mg and F, would appear to be a candidate. After we have established the dielectric properties of the  $BaMgF_4$ -SrMgF\_4 system, we plan to measure the dielectric properties at microwave and millimeter wave frequencies.

If additional time is available, we plan to add Sm<sup>2+</sup> to the crystals in various concentrations. The purpose is to study the line spectrum of Sm<sup>2+</sup> as a function of relative concentration of Sm and Eu and to study the interesting energy transfer from Eu<sup>2+</sup> to Sm<sup>2+</sup> in these materials. The dependence of the fluorescent lifetimes of the donor Eu<sup>2+</sup> ion and the acceptor Sm<sup>2+</sup> ion on concentration will provide evidence of the rates of energy transfer in these materials. In addition to the basic scientific interest, these measurements will provide information as to the feasibility of lasers prepared from these materials. Some of the energy transfer experiments can be done on powdered materials and some samples have already been prepared. If time permits, we also expect to conduct tests of x-ray sensitivity of these materials, and, if single crystals are available, some tests of scintillation counter efficiency will be undertaken.

# (b) Attempted Preparation of Ferromagnetic Oxides

Attempts to prepare ordered perovskites containing equal numbers of d<sup>3</sup> and d<sup>5</sup> transition metal ions, whose nearest-neighbor exchange interactions are ferromagnetic, have continued. Single-phase perovskite materials have been prepared in a narrow range of compositions around  $Ba_0._5Gd_0._5Mn^4+_0._5Fe^3+_0._5O_3$ , and the same composition, with  $Eu^3+$ replacing Gd<sup>3+</sup>, has been prepared. Magnetic susceptibility studies show the Eu compounds to undergo apparent antiferromagnetic ordering at 18°K, but the Gd compounds behave like paramagnetic materials down to 4.2°K. Mössbauer spectroscopy has been unsuccessful, owing to the high absorption by Ba and the rare earths for the 14 KeV gamma rays from <sup>57</sup>Fe. In both series of compounds, long-range magnetic ordering is either absent or very weak. A major difference between the two series of materials is seen in the behavior of the high-temperature dependence of the reciprocal susceptibility-temperature data. In the case of the Gd series, this curve extrapolates to zero at about -4°K, close to absolute zero, while the Eu compounds have an intercept at -120°K, indicating strong antiferromagnetic interactions between nearest Since the magnetic moment of Eu<sup>3</sup>+ is very small, this suggests that the magnetic coupling is dominated by antiferromagnetic and Fe-Fe interactions over the ferromagnetic Mn-Fe interactions. In short, these materials behave as if the Mn<sup>4+</sup> and Fe<sup>3+</sup> ions are disordered in the crystals.

On the other hand, the Gd series contain a rare earth ion with a high magnetic moment (S=7/2). This is close to the sum of the spin quantum numbers of Fe<sup>3+</sup> and Mn<sup>4+</sup> ( $\frac{5}{2} + \frac{3}{2} = \frac{8}{2} = 4$ ). If the net moment of the octahedral site ions coupled antiferromagnetically to the Gd ion moment, and no long-range magnetic ordering occurred, but the magnetic moments became frozen in random directions, we would observe the behavior described above. This has come to be known as "spinglass" behavior. Such behavior is characterized by the detection of hyperfine splitting in Mössbauer spectra, coupled with the absence of long-range magnetic ordering as observed by neutron diffraction.

Unfortunately, both Gd and Eu, the rare earths that formed these materials, have exceedingly high absorption cross-sections for thermal neutrons. The next rare earths, Tb and Dy, have high magnetic moments, and their nuclei are not strong neutron absorbers. Preliminary experiments to form perovskite phases have been unsuccessful.

will continue attempting the preparation We  $Ba_0$   $_5Tb_0$   $_5Mn_0$   $_5Fe_0$   $_5O_3$  and its dysprosium analog. Some effort will be placed on the use of low-melting fluxes such as  $BaO-B_2O_3$ , both for crystal growth and for enhancing the tendency of the atoms to assume an ordered arrangement in the structure. Preparation of the Gd compound using 57Fe-enriched starting material will be attempted in order to obtain a sample suitable for Mössbauer spectroscopy. Attempts will be made to prepare garnet phases where the octahedral sites contain d<sup>3</sup> ions such as Cr<sup>3</sup>+ while the tetrahedral sites contain Fe<sup>3</sup>+. Early attempts failed to get complete substitution of  $Cr^3+$  in the octahedral sites of  $Y_3Fe_5O_{12}$ , apparently because the  $Cr^3+$  ions are too small; we will attempt this in a garnet with a smaller unit cell, e.g.,  $YbFe_5O_{12}$  or  $LuFe_5O_{12}$ .

#### 4. PUBLICATIONS

- 1. E. Banks, Y. Okamoto and Y. Ueba, "Synthesis and Characterization of Rare Earth Metal-Containing Polymers. I. Fluorescence Properties of Ionomers," J. Appl. Polymer Sci., 25, 359 (1980).
- Y. Ueba, E. Banks and Y. Okamoto, "Synthesis and Characterization of Rare Earth Metal-Containing Polymers. II.
   Fluorescence Properties of Eu<sup>3</sup>+-Polymer Complexes Containing β-Diketone Ligand," J. Appl. Polymer Sci., 25, <sup>2</sup>007 (1980).
- 3. Y. Avigal and E. Banks, "Conductivity of Reduced Solid Solutions in the System Na<sub>2</sub>O-Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub>," Material Research Bulletin 15, 1381 (1980).
- 4. E. Banks, S. Nakajima and M. Shone, "New Complex Fluorides EuMgF<sub>4</sub>, and Their Solid Solutions: Photoluminescence and Energy Transfer," J. Electrochem. Soc., 127, 2234 (1980).
- 5. R. Sacks, Y. Avigal and E. Banks, "New Solid Electrolytes Based on Cubic ZrP<sub>2</sub>O<sub>7</sub>," J. Electrochem. Soc. 129, 726 (1982).
- 6. E. Banks, R. Jenkins and B. Post, "Crystal Structures of EuMgF<sub>4</sub>, SmMgF<sub>4</sub> and SrMgF<sub>4</sub>," presented at 15th Rare Earth Research Conference, Rolla, MO, 15 June 1981; manuscript accepted for publication in Conference Proceedings.

- 7. E. Banks, Y. Ueba and Y. Okamoto, "Lanthanide Ion Fluorescence as a Probe of Ionomer Structure," Annals of N.Y. Acad. Sciences 366, 356 (1981).
- 8. E. Banks and R Sacks, "ReP<sub>2</sub>O<sub>7</sub>: A New Isomorph of ZrP<sub>2</sub>O<sub>7</sub>," accepted for publication, Materials Research Bulletin.
- 9 Qiu Bingyi and E. Banks, "The Binary System SrF<sub>2</sub>-MgF<sub>2</sub>: Phase Diagram and Study of Growth of SrMgF<sub>4</sub>," accepted for publication, Materials Research Bulletin.

# 5. Dod and other interactions

- (a) Dr. J. S. Prener, General Electric R&D Laboratory, Schenectady, NY: interested in crystals of EuMgF $_4$  to use as scintillation counters in CAT scanners.
- (b) Professor R. Reisfeld and Dr. A. Loewenschuss of the Hebrew University, Jerusalem: collaboration on study of spectra of Sm+2 in the compounds explored in the JSEP work unit under laser excitation from 15°K to room temperature.

# F. ELECTRONIC PROPERTIES OF HYDROGEN IN SOLIDS

Professor D.C. Mattis

Unit SS2-6

#### 1. OBJECTIVE(S)

To develop first principles and theoretical techniques for relating the observed behavior of the hydrides of transition and rare-earth metals and their alloys to their underlying electronic properties. The mathematics will be applied to the bulk, surface and transport properties of these materials. A study of the broader question of the electronic properties of hydrogen in metals will be conducted.

#### 2. APPROACH

The behavior of hydrogen in solids is fast becoming one of the most important and unsolved problems of modern science. Despite astronomical efforts resulting in a vast body of mostly empirical knowledge, little has been achieved in the nature of comprehensive theory or an understanding that can be used for predictions. Currently, interest in the study of the electronic properties of hydrogenated solids is increasing, especially because of the existence of major unsolved problems whose resolution bears on the use of solids in electronic energy conversion and transmission. On a fundamental level, the electronic structure of defects lies at the forefront of current theoretical interest. Substitutional or interstitial hydrogen is one of the simplest possible solid-state defects, a near ideal testing ground for theories of impurities in solids. Its simple electronic structure also accounts for the many studies of its interaction with surfaces, catalysis and chemisorption. Recent theoretical work has laid the groundwork for attacking many of the important roles of hydrogen in solids from a fundamental point of view.

The combination of the approach of J. Friedel and co-workers, relating the observed behavior of transition metals to many-body effects, and methods developed by us for studying the response of interacting particles to various defects, will form the foundation for a theory of hydrogen in transition and rare-earth metals that has direct applicability to the many and startling effects observed in these systems. Ground state properties of the unperturbed metal system will be described by a variational Gutzwiller-type wave function, and schemes will be developed for applying modern techniques to the study of its excitation spectrum. The effect of hydrogen impurities is then treated by many-body perturbation theory of both the ground state and its excitations, in order to permit the description of time-independent and time-varying properties of the solids resulting from the presence of hydrogen impurities.

#### 3. PROGRESS

The main task within this unit during the past year has been an extensive investigation of the conditions under which a neutral hydrogen atom can bind to a positively charged particle. This problem is also that of an exciton trapped at a positive defect inside a solid, which represents one possible state of a proton within the solid. first analysis has shown that for such binding to occur, the mass of the positive particle, or hole, must exceed 1.46 of the mass of the free This is an important finding because it defines necessary conditions for the electronic properties of hydrogen in solids. first analysis used approximate wave functions for a three-body system related to those of the  $H_2^T$  ion. However, if the mass of the positive particle is comparable to that of the electron, its dynamic effects are also of the same order, and a many-particle wave function of both light particles, and sensitive to their interaction, is called for. The ground state of the system must be found by variational techniques that minimize the energy of the system with respect to several unconstrained The generalization of the first analysis to include these aspects is now under study, using different forms of the trial wave functions. A preliminary account of this work has already been given. 1 Additional publications that resulted from earlier work under this unit are also listed below. 2-4

Progress has also been made in extending Friedel's work on impurities in solids. In particular, we have extended the formulation to include situations in which the impurity has internal degrees of freedom such as a hydrogen molecule. The scattering of conduction electrons is, in this case, no longer an elastic process. The thermodynamic quantities can be expressed in terms of the imaginary part of the matrix. As J. Callaway<sup>5</sup> has pointed out, the t matrix is constrained satisfy the optical theorem

$$Im\{t(w)\} = -\pi \rho(w) |t(w)|^2$$

in which  $\rho(w)$  is the host density of states. Furthermore, the condition of charge neutrality forces the t matrix to be temperature dependent. These conditions severely restrict the form of the t matrix. A solution for the t matrix for a hydrogen impurity will allow all the thermodynamic properties to be ascertained.

Professor Mattis was granted a leave of absence for part of this period; however, his research on this unit has continued with the collaboration of a colleague and students, but with reduced effort.

#### 4. PUBLICATIONS

1. M. Farid and D.C. Mattis, "Does the Hydrogen Atom Bind a Proton?" Bull. Am. Phys. Soc. 26, 617 (1981).

- 2. R.E. Pena and D.C. Mattis, "Optical Lineshapes and Electronic Eigenstates of Substitutional Defects and Vacancies," J. Phys. C: Solid State Physics 14, 649 (1981).
- 3. A. Theumann, "Ferromagnetic and Spin-Glass Behavior in the Random Hierarchical Model," Phys. Rev. B <u>22</u>, 5441 (1980).
- 4. P.S. Riseborough and D.C. Mills, "Frequency Dependent Conductivity of the Anderson Lattice," in <u>Valence Fluctuations in Solids</u>, ed. L. Falicov, North Holland Publishing Co. (1981).
- 5. J. Calloway, Quantum Theory of the Solid State, Part B, Academic Press, N.Y., p. 386, (1974).

#### A. REDUCED-ORDER MODELS OF LARGE SCALE SYSTEMS

Professors D.C. Youla, F. Kozin and J.J. Bongiorno, Jr.

Unit IE2-1

#### OBJECTIVE(S)

Our objective is to produce reduced-order models for large-scale systems by a combination of time-domain, statistical and aggregation-like methods. The objectives can be divided into two major efforts.

- (1) Study and develop useful computationally stable and efficient order-reduction techniques. These techniques must yield good approximations of the dynamical quantities to be monitored.
- (2) Study and assess the effectiveness of reduced-order model control designs when applied to the original large scale system.

#### 2. APPROACH

Society is comprised of a multitude of large-scale systems. Communications, transportation, power, defense, waste disposal, and agriculture are but a few of the system substructures upon which our society is based. The heavy demands put upon these large systems by a society that continues to develop, as well as the desire to keep the systems themselves developing and operating in some reasonably efficient, safe, and cost-effective fashion, of necessity, requires intensive monitoring of each of the systems. However, the magnitude of these systems makes in-detail monitoring prohibitively costly even with current high-speed high-capacity computers. Reduced-order models, therefore, must be developed.

Problems to be studied for reduced-order models include: On what basis shall we construct a reduced-order model? What criteria shall be employed to arrive at a reduced-state model of the original system? What significant dynamical characteristics of large-scale systems can be predicted from lower-order models? Finally, how effective are design studies generated by lower-order models when applied to the original large-scale system? Parameters and state evolution may not be known exactly. Hence, there is uncertainty, either stochastic or deterministic, in our knowledge of the system. This fact must be accounted for in our development of order-reducing procedures, and their related computational algorithms. Thus, for example, the methods must be stable in the sense that small observation noise will not lead to large errors.

In our proposed research program, we shall be concerned with three major problem areas:

- (a) Analytical and computational methods for order reduction.
- (b) Applicability of control design concepts, generated from reduced-order models to the original large-scale system.
  - (c) Implementation to real large-scale systems.

#### 3. PROGRESS

The usual controllers for linear large-scale systems have been restricted to one-degree-of-freedom control methodology. As a result, it has been difficult to develop meaningful reduced-order models for such large-scale systems. During this past year, we have, by generalizing the permissible topology, developed a rigorous theory of two-degree-of-freedom controller design. We now present the background of the problem, derive some of the theoretical results, and present by example some of the exciting possibilities of this new theory.

# A. Introduction and Background

By and large, the design of optimal Wiener-Hopf controllers for linear large-scale time-invariant plants has been restricted to one-degree-of-freedom control laws. In turn, this has practically precluded the use of reduced-order modeling and has also made it impossible to incorporate other "hard" design specifications imposed by sensitivity constraints and phase-gain stability margin requirements, into a bonafide optimality theory.

In general, every control problem possesses two natural degrees of freedom: one corresponds to the availability of the exogeneous setpoint input u and the other to the availability of the sensor output w. However, in the conventional single-loop configuration, the controller generates the plant input r by processing only the difference u-w, and one degree of freedom is completely lost. To exploit the two inherent degrees of freedom fully, the controller must process u and w independently.

Now, apart from all other considerations, the design of a linear controller has two clearly defined objectives: one, the transient acquisition of a prescribed set-point input u(s) by the plant output v(s) must be accomplished satisfactorily in the presence of measurement noise v(s) and a saturation constraint on the plant input v(s); two, regulation of the face of load disturbance v(s) which enters through the plant must be acceptable. In the most general situation both requirements are present simultaneously, and the problem is one of servo-regulation. Available to the designer are the exogenous input v(s) and the feedback sensor output v(s) so that the overall configuration may be depicted schematically as shown in Figure 1.

To take advantage of both degrees of freedom, the controller can generate an output

$$\underline{r} = C_{u}\underline{u} - C_{w}\underline{w} \tag{1}$$

in which the two (open-loop) transfer matrices  $C_{\rm u}(s)$  and  $C_{\rm w}(s)$  may be shaped arbitrarily, subject solely to the demand of closed-system stability. On the other hand, because of its restrictive topology, the

<sup>(1)</sup> All matrix functions of the complex variable  $s = \sigma + j\omega$  are real and rational.

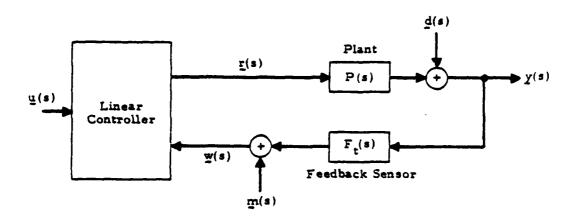


Fig. 1: General multivariable servo-regulator configuration

classical single-loop structure of Fig. 2 is able to process only the difference u(s)-w(s) and one degree of freedom is completely lost. It is therefore not surprising to find that under this limitation the two design objectives often conflict and appear mutually contradictory. Even worse, usually little or no latitude remains for the incorporation of sensitivity constraints and phase-gain stability margins. (2)

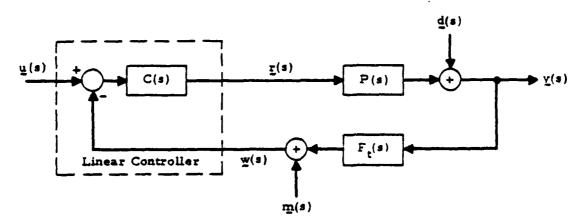


Fig. 2: The classical single-loop servo-regulator configuration

A primary goal of this year's research has been the development of a rigorous theory of two-degree-of-freedom optimal controller design which subsumes these additional design requirements into an overall analytic framework. Preliminary investigations indicate that such a theory may actually be within reach and a simple example presented in Section C reveals some of the exciting possibilities. Section B contains the necessary background material.

<sup>(2)</sup> The text by I. Horowitz<sup>1</sup> is notable for its appreciation of many of these factors.

# B. The Pure Two-Degree-of-Freedom Servo Problem

In Fig. 1 the transfer matrices P(s) of the plant and  $F_{t}(s)$  of the feedback sensor are prescribed and

$$T_{c}(s) = [C_{u}(s) - C_{w}(s)]$$
 (2)

is the desired controller transfer matrix from inputs u(s), w(s) to r(s). By straightforward analysis we obtain

$$\underline{r} = R_{u}\underline{u} - R_{w}(F_{t}\underline{d} + \underline{m}) , \qquad (3)$$

where

$$R_{u} = (1 + C_{w}F_{t}P)^{-1}C_{u}$$
 (4)

and

$$R_{w} = (1 + C_{w}F_{t}P)^{-1}C_{w} . (5)$$

Evidently,  $R_u(s)$  and  $R_w(s)$  are <u>closed-system</u> transmission matrices from exogenous inputs u(s) to r(s) and r(s) to r(s), respectively.

Let  $G_e(s)$  denote the spectral density of the error

$$\underline{e}(s) = \underline{u}(s) - \underline{v}(s) \tag{6}$$

and  $G_r(s)$  that of r(s). Then, in the standard quadratic-cost setting,<sup>2</sup> transient error and saturation are accounted for by the functional  $E = E_t + kE_s$ , where<sup>(3)</sup>

$$E_{t} = \frac{1}{2\pi j} \int_{-j\infty}^{j\infty} Tr G_{e} ds$$
 (7)

is the cost incurred by transient acquisition of u(s) and

$$E_{s} = \frac{1}{2\pi j} \int_{-j\infty}^{j\infty} Tr (Q G_{r}) ds$$
 (8)

is the penalty for excessive excursions in plant input r(s). The adjustable nonnegative constant k permits tradeoff between  $E_t$  and  $E_s$ , and Q(s) is a suitably chosen nonnegative-definite parahermitean weightmatrix. (4) Let the respective spectral densities of u(s), d(s) and m(s) be denoted by  $G_u(s)$ ,  $G_d(s)$  and  $G_m(s)$ .

<sup>(3)</sup> Tr  $A \equiv \text{trace } A$ .

<sup>(4)</sup>  $Q(s) = Q_*(s) \equiv Q'(-s)$  and  $Q(jw) \geq 0$  for all real w. (The prime denotes matrix transpose.)

For the pure servo problem with negligible sensor noise,  ${\rm G}_{\dot d}(s)$  and  ${\rm G}_{\dot m}(s)$  are both zero and the total cost is given by

$$E = \frac{1}{2\pi j} \int_{-j\infty}^{j\infty} Tr[(1 - PR_u) G_u(1 - PR_u)_* + kQR_u G_u R_{u*}] ds .$$
 (9)

Thus, we are led to the following definition.

<u>Definition 1</u>:  $R_u(s)$  is said to be <u>acceptable</u> for  $(P,F_t)$  if there exists a controller which realizes  $R_u(s)$  as the designated closed-system transmission matrix in an asymptotically stable configuration of generic type shown in Figure 1.

Clearly then, in the minimization of E, Eq. (9), only acceptable  $R_u$ 's qualify as admissible candidates and their parametrization is an important first step. Note also that our definition of acceptability does not restrict the controller to be dynamical, so that  $T_c(s)$  need not be proper. Some reasons for lifting this constraint have already been offered in reference 2, but, as a rule, optimal designs usually exhibit this property automatically. In any case, the matter can always be investigated after the parametrization of the larger class of acceptable  $R_u$ 's.

Assumption 1: The plant and feedback sensor are free of unstable hidden modes,  $F_t(s)$  is analytic in Re  $s \ge 0$ , and the <u>finite</u> pole of P(s) and  $F_t(s)P(s)$  in Re  $s \ge 0$  coincide and have identical McMillan degrees.

Except for the analyticity of  $F_t(s)$  in Re  $s \ge 0$ , all parts of assumption 1 are necessary for the existence of a stabilizing controller.<sup>2</sup> Let

 $A^{-1}B = F_{+}P = B_{1}A_{1}^{-1} \tag{10}$ 

where (A,B) is any left- and (B<sub>1</sub>, A<sub>1</sub>) any right-coprime pair of polynomial matrices. There exist<sup>1/2</sup> polynomial matrices X(s), Y(s),  $X_1(s)$ ,  $Y_1(s)$  such that

$$AX + BY = 1$$
,  $X_1A_1 + Y_1B_1 = 1$  (11)

and

$$\det X \cdot \det X_1 \not\equiv 0 . \tag{12}$$

Theorem 1 (New): Under assumption 1,  $R_u(s)$  is acceptable for  $(P,F_t)$  iff  $R_u(s)$  and  $P(s)R_u(s)$  are both analytic in  $Res \ge 0$ . Equivalently,  $R_u(s)$  is acceptable iff it is of the form

$$R_{11}(s) = A_1(s) H_{11}(s)$$
 (13)

where  $H_{ij}(s)$  is any matrix analytic in Re  $s \ge 0$ .

Hence, to minimize E we replace  $R_u(s)$  in (9) by (13) and vary over the free parameter  $H_u(s)$  analytic in Re  $s \geq 0$ ; optimization therefore fixes  $R_u(s)$  but not  $C_u(s)$  and  $C_w(s)$  individually, as is seen from Eq. 4. This latitude enables the designer to satisfy other requirements without sacrificing optimality. To make further progress it is necessary to introduce three additional assumptions which appear absolutely indispensable.  $^2$ 

Assumption 2:  $AG_uA_*$ ,  $A_{1*}(P_*P + kQ)A_1$  and Q are analytic and nonsingular on the finite  $s = j\omega$ -axis.

Assumption 3:  $(F_t - 1)P$  is analytic on the <u>finite</u> s = jw-axis.

Assumption 4: The spectral density  $G_u(s)$  vanishes at least as fast as  $1/s^2$  as  $s \to \infty$ , i.e., (5)

$$G_{ij}(s) \le O(s^{-2}) \qquad . \tag{14}$$

Theorem 2 (New): Suppose that assumptions 1-4 are satisfied and we let  $\Lambda(s)$  and  $\Omega_w(s)$  denote the Wiener-Hopf spectral solutions (6) of the two equations

$$A_{1*}(P_*P + kQ)A_1 = \Lambda_*\Lambda$$
, (15)

$$G_{\mathbf{u}} = \Omega_{\mathbf{u}} \Omega_{\mathbf{u}\mathbf{x}} . \tag{16}$$

Let

$$\Gamma = \Lambda_{*}^{-1} A_{1*} P_{*} \Omega_{11} . \tag{17}$$

Then, the unique acceptable design that minimizes E is given by (7)

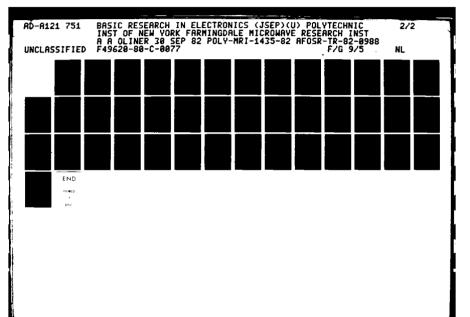
$$R_{u} = A_{1} \wedge^{-1} \{ \Gamma \}_{+} \Omega_{u}^{-1} \tag{18}$$

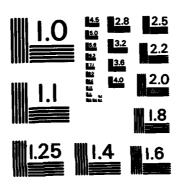
Comment: The compactness of (18) is somewhat deceptive because it depends both explicitly and implicitly on the coprime polynomials  $A_1(s)$  and  $B_1(s)$ . It is obviously desirable to eliminate these factors from all final formulas whenever possible.

<sup>(5)</sup>  $A(s) \le O(s^{\mu})$  means that no entry in A(s) grows faster than  $s^{\mu} + s \to \infty$ .

<sup>(6)</sup>  $\Lambda(s)$  and  $\Omega_{\rm u}(s)$  are square real rational matrices and  $\Omega_{\rm u}(s)$  with their inverses in Re s > 0; they are uniqued a to constant orthogonal matrix multipliers S

<sup>(7)</sup> In the partial fraction expansion of test the all the finite poles in Re  $s \le 0$  is denoted to analytic in Re  $s \ge 0$  and  $\le 0(1/s)$ .





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Corollary 1: Let P(s) be free of finite poles in Re s>0 and let  $\Lambda_r(s)$  denote the Wiener-Hopf spectral solution of the "reduced" equation

$$P_*P + kQ = \bigwedge_{r} \bigwedge_r . (19)$$

Then, under the conditions of Theorem 2, the optimal design is given by

$$R_{u} = \Lambda_{r}^{-1} \{\Lambda_{r*}^{-1} P_{*} \Omega_{u}\}_{+} \Omega_{u}^{-1}$$
 (20)

and all coprime factorizations are by-passed.

This corollary to Theorem 2 has a very wide range of practical applications because the number and location of the jw-axis poles of P(s) are totally unrestricted. These "infinite gain" frequencies play an important role. For example, good scalar servo design utilizes a pole of P(s) at s=0 to produce a system that can track a shape-deterministic step-input with zero steady-state error. More generally, in the multivariable case, a design preserves the steady-state acquisition potential of the plant if every finite jw-axis pole of P(s) is a zero of the determinant of the error transmission matrix  $1 - P(s)R_u(s)$  of sufficiently high multiplicity.<sup>2</sup>

Corollary 2: Any acceptable design  $R_{\rm u}(s)$  whose associated cost E is finite preserves the steady-state acquisition potential of the plant. A fortiori, so does the optimal design (18).

# C. An Example

A single-input-output plant has the transfer function

$$P(s) = \frac{s-1}{s(s-2)}$$
 (21)

Under the conditions  $k = Q(s) = F_t(s) = 1$ , use Theorem 2 to design a servo that tracks a step-input u(s) with spectral density  $G_u(s) = -1/s^2$ , optimally. (Sensor noise is negligible.)

Solution: Assumptions 1-4 are satisfied

$$A = A_1 = s(s-2)$$
 ,  $B = B_1 = s - 1$  (22)

$$\Lambda = s^2 + \sqrt{7} s + 1$$
 ,  $\Omega_{u} = \frac{1}{s}$  . (23)

Thus (details omitted), (18) yields the optimal design

$$H_u = \frac{-1}{s^2 + \sqrt{7} s + 1}$$
,  $R_u = \frac{-s(s-2)}{s^2 + \sqrt{7} s + 1}$ ,  $E = 3.65$ . (24)

In any stable closed-system realization of  $R_{\rm u}(s)$ , the tracking error e = u-y = (1 -  $PR_{\rm u}$ )u where

$$1 - PR_{u} = \frac{s(s + (1 + \sqrt{7}))}{s^{2} + \sqrt{7} s + 1}$$
 (25)

Hence, because of the presence of the factor s in the numerator of (25), any such servo can track a step-input with zero steady-state error, as predicted by corollary 2.

The single-loop realization of  $R_{\mathbf{u}}(\mathbf{s})$  shown in Fig. 3 cannot work, since

$$R_{ij} = (1 + CP)^{-1}C$$
, (26)

$$C = R_u (1 - PR_u)^{-1} = \frac{2 - s}{s + 1 + \sqrt{7}}$$
 (27)

and stability is precluded by the Re s > 0 pole-zero cancellation between P(s) and C(s) at s = 2.

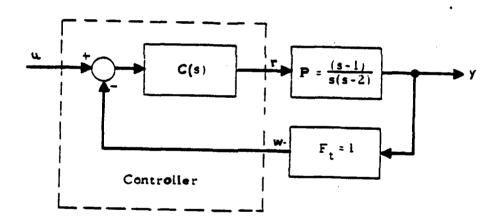


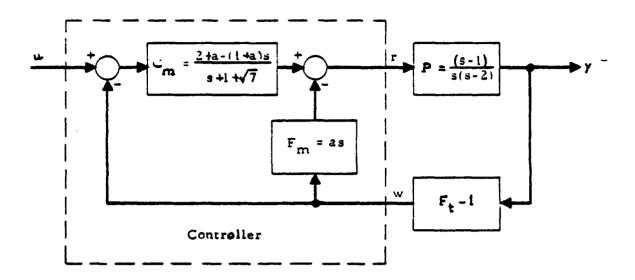
Fig. 3. Standard single-loop realization of the optimal design  $R_{ij}(s)$ .

However, if we insist on a single-loop topology, the smallest possible realizable cost is E = 131 which is achieved<sup>2</sup> by the design

$$R_{u} = \frac{s(s-2)((11 + 4\sqrt{7})s-2)}{(s+2)(s^{2} + \sqrt{7} s + 2)}, \quad C = \frac{(11 + 4\sqrt{7} s)-2}{s-(7 + 3\sqrt{7})}. \quad (28)$$

To accept this design is to accept an <u>unnecessary</u> 36-fold degradation in performance! (8) Actually, the cost E = 3.65 is easily attained by means of minor-loop rate-feedback around the plant (Fig. 4).

<sup>(8)</sup> The degradation is even more dramatic for k > 1.



$$C_m = C_u$$
;  $C_m + F_m = C_w$ 

Fig. 4. Realization of the cost E = 3.65 with minor-loop feedback.

To ensure closed-system stability, the gain constant a must be restricted to lie in the interval

$$-2 < a \le -1 , \tag{29}$$

and the obvious midpoint candidate a = -1.5 corresponds to the first-order lag compensator

$$C_{\rm m} = \frac{1+s}{2(s+1+\sqrt{7})} \tag{30}$$

But as is shown in Fig. 5, one can also achieve the cost E=3.65 by introducing additional compensation in the feedback path of the single-loop configuration of Figure 3.

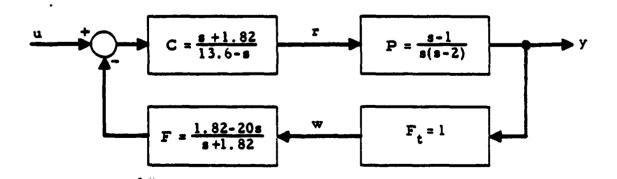


Fig. 5. Modified single-loop realization of the cost E = 3.65.

Evidently, to decide between the two designs, other criteria must be invoked.

The results of a detailed study of the sensitivity of the input-output transfer function  $T(s) = P(s)R_u(s)$  may be summarized briefly as follows. (9)

- 1) From 0 to 83.57 Hz, the sensitivity of T with respect to F in Fig. 5 exceeds that of T with respect to F<sub>m</sub> in Figure 4. In particular, over the range 0 to 11.44 Hz, it exceeds it by at least 17.3 db!
- 2) From 0 to 42.73 Hz, the sensitivity of T with respect to P (to C) in Fig. 5 exceeds that of T with respect to P (to  $C_m$ ) in Figure 4.

Since the 3-db bandwidth of T(s) is less than 6.28 Hz, it is concluded that the minor-loop design of Fig. 4 offers better sensitivity performance with respect to all parameters of interest. (10) Nevertheless, we are not suggesting that the minor-loop structure is invariably superior: On the contrary, the subject is wide open, especially in the multivariable case!

The cost-functional E, Eq. (9), does not depend on  $R_{\rm W}(s)$  and the latter must therefore differ for the two designs. Explicitly, for Figure 4, (11)

$$R_{W} = \frac{-s(s-2)(1 - (2 + 3\sqrt{7})s - 3s^{2})}{(s+1)(s^{2} + \sqrt{7} s + 1)}$$
(31)

while for Fig. 5,

$$R_{W} = \frac{-s(s-2) (1.82 - 20s)}{(s^2 + \sqrt{7} s+1)(s + 1.82)}$$
(32)

Over the bandwidth of the plant, the ratio of the magnitude of (31) to that of (32) reaches a maximum of  $\cong$  6, but for large  $\omega$  it grows without bound. Apparently then, the different sensitivity behavior exhibited by the two designs is intimately related to the different choice of closed-system transmission function  $R_{\omega}(s)$ .

$$R_{\mathbf{w}} = R_{\mathbf{u}} \cdot \frac{C_{\mathbf{w}}}{C_{\mathbf{u}}}$$

<sup>(9)</sup> a = -1.5.

<sup>(10)</sup> In our opinion, the improperness of the minor-loop compensator is of no great practical consequence.

<sup>(11)</sup> In Fig. 4,  $C = C_m$  and  $C_m + F_m = C_w$  but in Fig. 5,  $C = C_u$  and  $CF = C_w$ . Thus, (31) and (32) are obtained by using the formula

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# 5. Dod and other interactions

- (a) Under an arrangement that the Rome Air Development Center, New York, has with Syracuse University, New York, known as SCEE, Professor Youla has performed consulting work for Dr. Heywood Webb of RADC each summer for the past three summers. The topics which he first explored under JSEP sponsorship, were: Engineering applications of the Prony technique; Recovery of spectral information from analogue covariance data; and Diagnostics for nonuniform media.
- (b) On an extension of work originally supported by JSEP, Professor Youla has recently had a contract with RADC on the topic of image restoration.
- (c) Professor Youla was invited to present a talk on his new theory of spectral estimation, developed under this work unit, at the meeting on "Techniques of Spectral Estimation," held at the Naval Postgraduate School, Monterey, California, during 1980, and sponsored by the Office of Naval Research. Many Navy researchers were present, and very good interaction resulted with Professor Youla concerning their special problems.
- (d) Professor Youla was invited to present talks on the subject of spectral estimation at Texas Tech and at the University of Maryland.

# B. ENHANCEMENT, EXTRACTION AND RECONSTRUCTION TECHNIQUES IN IMAGE PROCESSING

Professors A. Papoulis and L. Kurz

Unit IE2-2

#### 1. OBJECTIVE(S)

The main purpose of this research effort is to investigate some new and promising approaches to the general problem of image enhancement, extraction, and reconstruction. The investigation will encompass two philosophically different classes of techniques: spectral-estimation and statistical.

In connection with the spectral-estimation approach, it is proposed to develop a new method of filtering, combining frequency domain techniques with the advantages of adaptive and recursive estimators. The method is based on the representation of an arbitrary signal f(t) in terms of the samples of its "running FFT," and it can be used without any knowledge of prior statistics. A special form of the filter leads to an extension of the gradient-seeking algorithm used in a variety of LMS estimators. The study will include the development of the properties of running transforms and their use in spectral estimation.

The statistical class of techniques includes the study of several types of statistical masks, edge detection procedures, and image reconstruction algorithms. In addition, feature extraction and object identification based on various versions of factor analysis techniques will be studied.

The prime objective of the research effort is to obtain general results with broad implications in such areas as interpretation and classification of pictorial data, processing of radar data of all forms, geological and underwater sounding, meterological and oceanographic data, space and communications data, etc. Whenever feasible, comparative studies of the two classes of approaches for a given application will be attempted.

Among others, the following aspects will be considered: various features of image processing with emphasis on noise and clutter reduction; detection of quasimonochromatic sonar signals in the presence of echoes and engine interference; rapid measurement of the instantaneous frequency of FM signals; adaptive equalizers; recursive estimation of covariance matrices.

# 2. APPROACH

The two different basic approaches are discussed separately in the presentation below.

# A. Spectral-Estimation Approach

To place the proposed spectral method into familiar perspective, we shall relate one of its applications to adaptive LMS estimation. We shall use as an illustration the estimation of a discrete process y[n] in terms of the output:

$$\hat{y}[n] \sum_{k=0}^{N-1} a_k[n] \times [n-k] = X^T[n] A[n]$$
 (1)

of a non-recursive time-varying filter of length N with data process X[n] as the input. Our objective is to determine the weights  $a_k[n]$  so as to minimize the MS value of the estimation error.

$$e[n] = y[n] - \hat{y}[n]$$
 (2)

If the statistics of the process x[n] and y[n] are known, then (Wiener filter)<sup>3</sup>

$$A[n] = R^{-1}\Gamma \tag{3}$$

where

$$R = E\{X[n]X^{T}[n]\} \qquad \Gamma = E\{X[n] \quad y[n]\}$$
 (4)

In the absence of this information, we can either estimate the covariance matrix R and the cross-covariance vector  $\Gamma$ , or we can determine A[n] adaptively. A simple method of adaptaion based on an instantaneous version of a gradient-seeking technique for minimizing the MS error is the algorithm

$$a_k[n+1] = a_k[n] + \mu e[n] x[n-k]$$
 (5)

introduced by Widrow<sup>1,4</sup> and used in several areas of signal processing.<sup>5</sup>

The Widrow filter is simple; it requires no prior knowledge of any statistics, and it can be applied to stationary and non-stationary processes. It has, however, a number of disadvantages: The number N of coefficients that are adaptively controlled equals the length N of the filter. This often introduces unnecessary complications if N is large. Filtering of noise is best performed in the frequency domain. This leads to a small number of unknown parameters if they control directly the frequency response to the filter. The solution of (5) is a random set of weights A[n] that does not approach the Wiener optimum<sup>6,7</sup> [see (3)]. The estimation can be simplified if the adaptively controlled coefficients are associated with nearly uncorrelated data (Karhunen-Loeve). This is not the case, in general, with the data x[n-k] in (1). The length N of the filter is fixed; this is often undesirable.

In last year's Annual Report, an approach was presented which overcomes these difficulties, but the details will not be repeated now.

# B. Various Statistical Approaches

The masking techniques and techniques based in ANOVA (analysis of variance) used by the senior investigator (Professor Kurz) in the past were unified within the framework of the statistical linear models. In a basic paper, 8 he introduced a collection of simple procedures based on masks to be used in computer image processing. Small, carefully selected regions of an image are viewed at one time. The process is repeated throughout the image. Many different types of masks were introduced which accomplish efficiently the tasks of edge detection, noise reduction, shrinking, expansion, object recognition, measuration, etc. In a separate paper<sup>9</sup> the effectiveness of ANOVA techniques were Simultaneously, demonstrated in image processing and enhancement. classes of Robbins-Monro type stochastic approximation minimum variance least squares (SAMVLS) estimators were developed 10,11,12 for which the resultant regression function is interpreted as a recursive correlator. Robustness (relative insensitivity) to variations distribution and insensitivity to contamination of data is achieved by batch preprocessing of the data either by using linear rank tests (batch-nonlinear-linear or BNL approach) or by using adaptive gain coefficients with properly preselected nonlinearity. By combining the theory of ANOVA, experimental design and robustized SAMVLS, new three-dimensional recursive masks were introduced for real-time parallel processing and detection of stationary or moving images in unspecified noise environment from observations taken of a noisy scene. The method has the potential for development of techniques for estimation of velocity and acceleration of moving objects. In addition, the theory of Latin Square experimental designs is particularly attractive as an approach to the design of three-dimensional masks.

In a separate paper, 13 it was demonstrated that two-dimensional partition tests are effective in achieving excellent quality edge detection in the presence of severe and undefined noise. The philosophy of this approach needs further extension to include nonlinear processing which is particularly useful in the processing of images appearing in radar and underwater sounding data. The extended model should include the problem of moving objects, velocity, acceleration, etc.

Using masking techniques in conjunction with occupancy vectors of partition tests represents an interesting marriage of the two approaches outlined above. The full impact of this hybrid version of image processing problems is not clear at this time but preliminary results indicate its potential for efficiently solving numerous problems in image processing.

Two classes of recursive factor analysis techniques as a means of achieving feature extraction and image identification were introduced in reference 15. This approach is particularly useful in processing massive arrays of data. Further development and refinement of this approach will result in the attainment of an efficient software library for reducing and identifying severely corrupted and/or unknown images imbedded in an unknown background noise.

### 3. PROGRESS

Progress will be reported separately for the spectral estimation and statistical approaches.

# A. Spectral Estimation Approach

During the contract period, we have treated the following problems.

# (1) A new approach to the bandlimited extrapolation algorithm

The extrapolation algorithm introduced earlier 16'17 for the reconstruction of finite objects in terms of their diffraction limited images, is effective primarily for point sources. 18'19 For extended objects, the convergence is slow and the results are strongly affected by noise. To eliminate these problems, we have introduced a modification of the algorithm based on a new iteration whose limit is no longer bandlimited but whose transform is close to the aperture field of the unknown object. By a suitable selection of the iteration parameters, we achieve a balance between accuracy of image restoration and noise effects. We are in the process of testing the method numerically.

# 2. Application of running FTT's

The method of running FFT's developed earlier<sup>20</sup> has been applied to a variety of problems involving filtering and image restoration. Recent results involve the application of the method to the problem of detecting a target in the presence of strong clutter. We have developed a time-varying filter whose parameters are adaptively controlled according to the local statistics of the environment. The processing is carried out in the frequency domain and the cut-off frequencies of the filter are estimated with various threshold techniques. Unlike other methods, this approach does not assume prior knowledge of background statistics. The method is particularly effective for the clutter reduction problem because the filtering is carried out directly in the frequency domain.

To improve the effectiveness of the method, we are currently considering prediction techniques based on focal plane processing.<sup>21</sup>

# (3) Maximum entropy

We have considered various aspects of spectral estimation based on the method of maximum entropy. Our results center on the following two areas: (a) A critical examination of the method and its relationship to the Wiener theory of prediction, autoregressive processes, the Levinson algorithm, lattice filters, all-pole and all-pass systems, and stability.<sup>22,24</sup> (b) Reexamination of the method based on prior information about the bandwidth of the unknown spectrum. Introduction of windows<sup>23</sup> for reducing the effects of oversampling and the presence of spurious lines in the all-pole estimate of the unknown spectrum.

All three of these areas are under continuing investigation. Under references and publications we shall record results that are near completion or are already accepted for publication or presentation.

On bandlimited extrapolation: A modification of the algorithm introduced in reference 43 resulted in a paper (reference 38, to appear). The paper involves a novel method for estimating a bandlimited signal in terms of a single sample contaminated by noise, under energy constraints.

On the adaptive frequency domain technique: In the generally used algorithm

$$a_k[n] = a_k[n-1] + \mu \bar{\epsilon} [n] \bar{x} [n-k]$$

 $\bar{x}[n]$  and  $\bar{\epsilon}[n]$  are truncated versions of the data x[n] and the error  $\epsilon[n]$  and the truncation levels are unequal. We show that this might lead to instabilities if the signal contains periodic components, and we examine the stability conditions. A paper is in preparation.

The FM applications include the determination of the spectral properties of stochastic FM signals. The results are reported in papers 37 and 42. On spectral estimation: A method is being developed for estimating the parameters  $\lambda_0$  and  $\gamma$ i of the spectrum  $S(\omega)$ . The method is based on the properties of the roots of the error polynomial  $E_N(z)$ . If, in Levinson's algorithm,  $|\gamma_M|=1$  and  $|\Gamma_N|<1$  for N< M, then all roots of  $E_N(z)$  are on the unit circle and all roots of  $E_N(z)$  are inside the unit circle for N< M. This is used to estimate the number of lines in  $S(\omega)$  and the unknown parameters. Preliminary results are reported in paper 36.

# B. Various Statistical Approaches

In connection with the work on statistical approaches to the problems of image enhancement, extraction and reconstruction, several important new results were obtained and some of the past results were extended and sharpened.

earthsounding images result (1) Radar, sonar and particularly weak signals. In addition, the underlying distributions in the latter class of problems are poorly defined. Faced with these difficulties, numerous investigations in this area concentrated their research efforts on array processors, preferably of the robust type. 26,27,28 In the last year some new results in this area were presented in a paper. 25 The typical assumptions of gaussianity and stationarity of additive noise were removed. In addition, it was assumed that the noise at the sensor inputs are inter-correlated. To robustize the array processing procedure, the optimal nonlinearities at the correlator's inputs were approximated by simplified nonlinear functions based on parameters which can be easily estimated. The effect of the inter-sensor noise dependence on the asymptotic relative efficiency (ARE) of a multiple-input correlation detection procedure was examined. Easy to implement detector realizations were shown to be efficient when compared with the optimum detector configurations.

- (2) Object reconstruction algorithms, <sup>29</sup> extraction of moving objects by recursive parallelepiped masks<sup>30</sup> and edge detection using Latin Square masks<sup>31</sup> depend strongly on a good robust recursive vector parameter estimator. A refined version of such an estimator was generated: <sup>32</sup> An improved rate of convergence, guaranteed low variance of estimation and high degree of robustness (insensitivity to variations in underlying noise distributions) result from the use of ranktype preprocessors. The latter class of preprocessors act as efficient guassianizers of poorly conditioned data.
- (3) The statistical mask procedures presented in references 30 and 31 may be considered as belonging to a class of masks based on experimental designs. Another important class of problems was that of trajectory detection, which may also be treated using statistical masks based on theory of experimental designs. In particular, masks based on the symmetrical balanced incomplete block designs (SBIB) were studied in detail.

A trajectory is identified by a continuous and narrow region of high intensities which is surrounded by a region of low intensities on each side. When an image containing such a trajectory is processed by a localized operator (window or mask), the grey level distribution within the mask behaves like either a pulse function or a step function, depending on whether the mask is placed perpendicularly or in parallel to the trajectory. The traditional square-shaped edge detector is ineffective in this application regardless of the relative position of the mask to the trajectory. A small edge detector may not contain enough variations due to trajectory elements to cause significant block effects. On the other hand, a large edge detector may cover too wide an area so that adjacent trajectory segments are included in the same mask. What is needed is an experimental design in the shape of a stretched rectangle. When this design is placed perpendicularly to the trajectory, it allows for inclusion of three component parts of a pulse function. When the mask is placed in parallel to the trajectory, it allows for the inclusion of substantial elements from only one trajectory segment to form a step function.

A trajectory is further characterized by two inherent properties: the block nature and strong contrast of trajectory elements. Firstly, the elements of the actual trajectory tend to be adjacent to one another. Their grey level or texture tend to be similar when compared with the surrounding elements on both sides of the trajectory. Secondly, the grey level distribution changes drastically on both sides of the Thus only those block effects which are associated with trajectory. strong contrast can be considered as indicative of a "true" trajectory. Based on these properties, image data can be considered as a three-dimensional array with the row and column number describing the planar position and the grey level distribution being described by the third dimension. In terms of experimental designs, the analysis of an image containing a trajectory calls for a model which can determine the presence of row, column or grey level effects independently. An SBIB design satisfies all the required conditions: it is shaped as a stretched rectangle, its analysis determines if there exist significant block or

grey level effects independently, and the adjusted block means can be used as unbiased estimators of the true block means. In its application to the trajectory detection problem, the hypothesis that a SBIB mask contains a trajectory portion is accepted if the following three conditions are satisfied simultaneously: (a) there exist significant block effects; (b) there exist significant grey level effects; (c) the adjusted block means behave like a pulse function. To satisfy the randomization criterion, a SBIB design is selected from a set of existing designs randomly and then its grey level designations are further randomized by permutations of the row and column assignments. The first two conditions can be easily implemented by comparing the F statistics of a SBIB design to a threshold value corresponding to a preselected confidence level. The shape of the grey level distribution can be determined by thresholding the adjusted block means by their overall means.

The ideas outlined above have been implemented and found to produce excellent results even if the trajectories are severely corrupted by noise. A research paper based on these ideas is in preparation and should be submitted for publication in the fall of 1982.

(4) Detecting edges separating grey levels is an important aspect of image processing. A new procedure for detecting edges based on radial F-statistics has been developed in the last year. Though the procedure is uniformly most powerful (UMP) for a gaussian noise background, 33 it remains robust (insensitive to changes in noise distribution) in many situations. 4 If conditions of reference 34 are not satisfied, robustness of the procedure may be achieved using robustizing algorithms developed in references 29 and 32. The actual detection method is based on the use of F-statistics along radial vectors from inside of the object enclosed by the edge. To find the location of a region inside an object, several simple procedures to accomplish this task have been generated. It was shown that the radial F-statistic along a vector beginning inside an object varies linearly between two constant values in passing between two grey levels. The midpoint of the linear portion represents a true edge point. The pertinent F-statistic is of the form

$$F_{i,m} = \frac{V_i^2}{V_t^2} = [\frac{1}{m} \sum_{i=1}^{m} (S_i - \sum S_i/m)^2] / [\frac{1}{m} \sum_{i=1}^{m} (S_{ti} - \sum S_{ti}/m)]$$

where  $V_i^2$  = sample variance of the extracted sample,  $V_t^2$  sample variance of the training sample and the notation of reference 35 has been used. The ideas outlined above have been thoroughly tested on various corrupted images yielding excellent results. The final version of the paper based on these ideas is in preparation.

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# C. ROBUST PROCEDURES IN ESTIMATION AND DETECTION PROBLEMS

Professor L. Kurz

Unit IE2-

# 1. OBJECTIVE(S)

Considerable interest generated in robust estimation and detection problems motivated the development in recent years by the senior investigator in cooperation with his doctoral students of several classes of rank and non-rank detection procedures as well as robust estimation procedures which use nonparametric preprocessors to achieve a high degree of robustness in the presence of unknown noise and/or severe extraneous contamination of the data. The main objective of future research is to concentrate the effort on classes of detectors based on mixed statistics which preserve excellent qualities of rank and non-rank procedures; also included in the effort will be the imposition of side constraints, statistical dependence, sequential modes of operation and array processing of the data. A parallel effort will include extensions of the robustized estimation techniques to problems involving stochastic approximation minimum variance least squares estimators (SAMVLS) and Kalman-type estimation and filtering problems. The interaction of the robust detection and estimation techniques in adaptive systems will be studied. Particular attention will be given to the application of the procedures to problems in radar, sonar and communications.

### 2. APPROACH

The statistical properties of partition detectors and their variants are well understood. A concise exposition of the present state of the art may be found in reference 1. The mathematical framework introduced therein permits a logical evolution of many robust detectors with an almost inexhaustible source for developing such detectors useful in various applications. In addition, two approaches introduced in a recent paper of ours<sup>2</sup> for including side constraints in the design of robust detectors represent a major step in our ability to evolve many flexible procedures for robust detection subject to various physical constraints. Inclusion of statistical dependence and sequential modes of operation<sup>2,3,4,10</sup> adds another important dimension to the utility of partition detectors. The interaction of the approaches outlined above represents an almost inexhaustible source for solving numerous interesting and useful problems involving detection of weak signals in an unknown environment.

In a recent paper,<sup>5</sup> a new class of non-rank robust detectors, which are related to the generalized quantile detector<sup>1</sup> was considered. Unlike the non-rank detectors based on quantile statistics with fixed scoring vectors, the new class of detectors uses a random scoring vector. This new class of detectors is particularly useful in a noise environment that is relatively rapidly-varying.

The approach to robust recursive estimation problems initiated in references 6 and 7 with its extensions presented in references 8 and 9 represents another source of numerous theoretical and practical problems of interest in radar, sonar and communications. Inclusion of statistical dependence and other constraints in this approach will yield a tool of almost limitless potential for solving practical estimation problems when the parameters to be estimated are severely corrupted by noise or the noise is unknown or varying. Various additional forms of robustized estimators, including p.d.f., c.d.f., and score estimators, permit solution of numerous practical problems. For all approaches outlined above stress will be placed on procedures which are applicable in real-time processing and are simple to implement.

# 3. PROGRESS

- A. The results on dependent sampling in sequential partition detectors reported in reference 10 were extended to a more general model of Markov-dependent noise. <sup>11</sup> This paper involves proving certain basic theorems which point to the fact that considerable advantage in detection efficiency of partition detectors is achieved if one uses the Markov-dependent structure of noise. The results open the door to a whole new class of robust detectors which utilize the structure of dependence of the underlying noise to improve the efficiency of detection.
- The advent of modern high-speed sampling techniques result in additional stress on the problem of signal processing in dependent noise mentioned in the previous paragraph. Since in many systems of practical interest the knowledge of the noise statistics is either inexact or unspecified, some adaptive techniques which are frequently ineffective or too complicated to implement were suggested in the past. However, if one applies the methodology of system identification, the approach is essentially equivalent to the operation of a prewhitening filter. In particular, in a recent paper 2 a procedure for robust identification of the autoregressive (AR) model was introduced. The robustizing process is in the form of a robustized Robbins-Monro stochastic approximation (RMSA) algorithm and is based on the m-interval polynomial approximation method. The resulting algorithm represents a recursive robustized version of the well-known maximum entropy method (MEM) for spectral estimation introduced by Burg<sup>13</sup> or of the popular Widrow least-mean-square (LMS) adaptive filter.<sup>14</sup> Furthermore, the robustized algorithm leads naturally to a robustized Akaike's information criterion (AIC). 15 The simplicity of implementation and flexibility make the application of the new robust identification algorithm particularly attractive in practical applications. The flexibility and robustness of the new procedure were confirmed by extensive Monte Carlo simulations.
- C. The standard Kalman filter will usually diverge when the dynamic noise is not Gaussian. A robust Kalman filter based on minterval polynomial approximation (MIPA) method for nongaussian noise was formulated. Two situations were studied in detail: (a) the states are gaussian and the observation noise is nongaussian, (b) the states are nongaussian and the observation noise is gaussian. It was

shown that the MIPA Kalman filter maintains efficient performance over a broad class of noise distributions and is both computationally attractive and easy to implement. Compared to the min-max Kalman filters suggested by other authors, the new class of filters is more efficient and robust. The theoretical results were verified by extensive Monte Carlo simulations.

- D. A particularly efficient and flexible new approach to robust detection was introduced in reference 17. In the paper, the Huber-Tukey model of mixture distributions is replaced by a more versatile one which leads to solutions which are more appealing from a practical point of view than the robust detectors using the Huber-Tukey noise model in conjunction with the min-max criterion of performance. The new detector consists of two parts -- parametric and nonparametric -- which are switched in or out depending on one parameter of the mixture distribution model. As part of the detector, an efficient running estimator of this unknown parameter is included. When compared to the min-max detector proposed by other researchers, the new detector is more efficient for deterministic and stochastic signals. This divergence in efficiencies is particularly apparent under severe and/or variable noise conditions.
- Suppression of impulsive noise and timing jitter to robustize data transmission systems requires modification of signal selection and equalization processes. 18,19 A further contribution to this robustizing approach to equalization in data transmission systems was presented in two new papers. 20,21 In particular, the correlatively-coded signals tolerant to sampling offsets (timing jitter) described in reference 19 were recursively equalized at the receiver.<sup>20</sup> It was shown that for data transmission systems disturbed by noise, controlled intersymbol interference and sampling offsets, the recursive equalizer<sup>20</sup> yields improvement when compared to the nonrecursive equalizers.<sup>19</sup> In addition, the results of reference 18 were generalized to PAM systems using partial response techniques.<sup>21</sup> The results presented in the paper permit a meaningful study of practical systems because even if the nonlinearity is not added to the system to suppress impulsive noise, all real systems have a finite dynamic range of linear operation and act as soft limiters with a high saturation level. In particular, the effect of nonlinearities on intersymbol interference and signal shaping was considered. The generalization of the equalizer design in the frequency domain was presented resulting in suppression of degradation of system performance because of the nonlinearity in the system. Several partial response signals which are of interest in practical systems were con-Finally, comparisons between a standard PAM system and a partial response system in the presence of nonlinearities were given.
- F. The importance of data links discussed in the preceding section in computer-communication networks led naturally to the preliminary study of transition probabilities in such networks. To facilitate the generation of the pertinent transition probabilities, an approximate efficient technique was evolved in the paper. Using time-dependent coefficients and state-dependent orthogonal functions in a generalized Fourier series, approximate solutions to the pertinent Fokker-Planck

equation were generated yielding both transient and steady-state solutions to the problem. For a given mean-square error, the efficiency of the approximation is achieved by an appropriate choice of orthogonal functions which require the minimum number of terms in the series expansion. The small number of coefficients in the series are determined as solutions of a system of ordinary differential equations resulting in a high computational efficiency of the method. It should be noted that the procedure outlined in the paper is applicable in obtaining solutions to other than Fokker-Planck partial differential equations.

G. The theory of partition detectors was extended to so-called double-threshold detectors which are particularly useful in radar applications. Quantization loss of the commonly-used double-threshold detector is minimized by using a multi-level threshold for the first threshold. The overall performance is improved by optimal selection of partitions (thresholds) and scores. Expressions for false alarm rates and detection probabilities and upper bounds based on the generalized Chebysher inequality are presented. In radar applications the new detector performs better than detectors suggested by other researchers. The new detector has potential for application to communications through dispersive media.

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# 5. Dod and other interactions

- (a) The robust detection techniques developed by Professor Kurz have been of interest to the Navy in solving certain types of underwater sounding problems. His former students were involved with this problem at Bell Laboratories under a contract with the US Navy. In recent years, one of his students (Dr. Roger Dwyer, Underwater Sounding Laboratory, US Navy, New London, CT) in collaboration with him worked on applying statistical partition techniques to underwater sounding.
- (b) The work on statistical techniques and image reconstruction algorithms is of interest to the IBM Corp. They have published three internal research reports based on Professor Kurz' work in this area, and they hope to include these approaches in their future software packages.
- (c) At the recent IFIP Conference, Professor Kurz, was approached after his presentation by people from several agancies of the U.S. Government. The Bureau of The Census and the Department of Energy, in particular, asked him to give presentations to their staffs on his robustizing approaches to statistical inference.

# SECTION IV SIGNIFICANT SCIENTIFIC ACCOMPLISHMENTS

# Polytechnic Institute of New York Microwave Research Institute

# REPORT

on

# SIGNIFICANT SCIENTIFIC ACCOMPLISHMENTS

In this Report on Significant Scientific Accomplishments, we group separately the listings for the 1980-81 year and those for the 1981-82 year. For convenience, however, the numbering of the items is consecutive.

# Year ending September 30, 1982

1. Rigorous Solution for the Oblique Guidance of Electromagnetic Surface Waves by Periodically-Grooved Dielectric Waveguides, and Its Many Implications

Professors S.T. Peng and A.A. Oliner Work Units EM1-1 and EM1-4

2. Extension of Dynamical Theory to X-Ray Phonon Interactions

Professor H.J. Juretschke and Mr. F. Robbins Work Unit SS1-1

3. A Robustizing Approach to System Identification

Professor L. Kurz Work Unit IE1-3

4. Collective Approach to High Frequency Transmission of Electromagnetic Waves Through Dielectric Layers

Professor L.B. Felsen and Mr. P.D. Einziger Work Unit EM1-2

5. Optimal Multivariable Controllers Employing a Two-Degree-of-Freedom Design Methodology

Professors D.C. Youla and J.J. Bongiorno, Jr. Work Unit IE1-1

6. New Interpretation of Size Effects in the Conduction Properties of Thin Metallic Films

Professor H.J. Juretschke and Mr. R. Pimpinella Work Unit SS1-4

# Year ending September 30, 1982

7. Leaky Wave Theory for Dielectric Grating Antennas of Finite Width

Professors S.T. Peng and A.A. Oliner Work Unit EM2-1

8. Direct Phase Determination of X-Ray Structure Factors Using Reflected Intensities in the Renninger Geometry

Professor B. Post Work Unit SS2-1

9. Theory of Phase Information of X-Ray Structure Factors in the Asymptotic Intensities Near n-Beam Interactions

Professor H.J. Juretschke Work Unit SS2-1

1. Rigorous Solution for the Oblique Guidance of Electromagnetic Surface Waves by Periodically-Grooved Dielectric Waveguides, and Its Many Implications

Professors S.T. Peng and A.A. Oliner

When electromagnetic surface waves are guided by a periodically-grooved dielectric layer waveguide, and the waves propagate in a direction perpendicular to the periodic grooves, the TE and TM surface waves are not coupled and the boundary-value problem is a scalar two-dimensional one. When the surface waves are guided at an oblique angle to the grooves, however, TE-TM mode coupling occurs, and the problem becomes a formidable vector three-dimensional one. We have recently obtained a rigorous solution to the oblique guidance problem for a dielectric periodic waveguide with rectangular grooves. To our knowledge, this is first rigorous solution to a vector problem involving any kind of periodic structure.

The problem which was solved has great practical value and potential importance. First of all, it represents a structure which is currently being explored in integrated optics for applications such as multiplexing. Because of its potential for many other applications, careful measurements were made recently in Germany but there was no theory against which these measurements could be compared. Our theory provides excellent agreement with those measurements, which correspond to the Bragg region of the wavenumber plane, and which exhibited four stop bands instead of the ordinary two because of the added TE-TM mode coupling.

We have recognized that the solution we derived is also applicable to a variety of problems in the millimeter-wave integrated circuit field, in particular to periodic gratings on dielectric waveguides of finite width, for which no solutions are yet available. We are currently utilizing this solution in the analysis of two basic periodic grating structures of this type: (1) a grating whose dimensions place it in the Bragg reflection region so that it finds application as a resonator or filter; there, we find that an extra (unwanted) reflection peak or transmission dip is obtained, and (2) a grating whose dimensions permit leakage of radiation so that the structure becomes a leaky wave antenna. In the first example, we find a new effect which can seriously impair device performance; in the second example, our new solution permits the development of a theory for this class of antennas.

Our significant contribution here is that we have derived a rigorous solution which not only is the first of its type but also is a key to the opening of many new doors.

# 2. Extension of Dynamical Theory to X-Ray Phonon Interaction

Professor H.J. Juretschke and Mr. F. Robbins

The interaction of x-rays with many phonons has been formulated under the conditions for which both the primary and the scattered

x-ray modes consists of two or more coherently coupled plane waves. In addition, the scattered modes are treated as subject to boundary conditions appropriate to entirely internally generated fields. dynamically self-consistent theory predicts new features of x-ray phonon interaction under diffraction conditions, such as satellites in the main reflection, line narrowing and peak reduction beyond that of the Debye-Waller factor, and collective phonon-induced changes in the index of refraction of all the x-ray modes. Some aspects of these features have been seen in already published experiments. Others are below the resolution available under most presently employed experimental conditions, but they will become accessible with the appropriate use of synchrotron sources. The theory also contains the full description of the interaction of x-rays with photons in those solids where the photon propagates within the crystal in strong coupling to optical phonons the so-called polariton. This particular type of nonlinear interaction between x-rays and lasers in the optical range is the strongest and therefore the most likely to be experimentally observable. The observations predicted by our calculations will constitute a test of the extent to which current dynamical theory, which is self-consistent but is essentially a linear theory, can account for such interactions and also the extent to which a more microscopic theory of x-ray propagation in crystals has to be sought, especially as the intensities of such x-rays continue to increase.

# 3. A Robustizing Approach to System Identification

#### Professor L. Kurz

The advent of modern high-speed sampling techniques has resulted in additional stress on the problem of signal processing in a dependent corrupting noise. Since in many systems of practical interest the knowledge of the noise statistics is either inexact or unspecified, some adaptive techniques which are frequently ineffective or too complicated to implement were suggested in the past. If the methodology of system identification can be adjusted appropriately, a process equivalent to the prewhitening filter may be evolved. To that end, a robust identification of the autoregressive (AR) model was introduced.

The robustizing process is in the form of a robustized Robbins-Monro stochastic approximation (RMSA) algorithm and is based on the m-interval polynomial approximation (MIPA) method proposed recently by the author. The resulting algorithm represents a recursive version of the well-known maximum entropy method (MEM) for spectral estimation introduced by Burg or of the popular Widrow least-mean-square (LMS) adaptive filter adopted in many engineering disciplines. Furthermore, the robustized algorithm leads naturally to a robustized version of Akaike's information criterion (AIC) to determine the order of the autoregression. The simplicity of implementation and flexibility make the application of identification algorithms based on the MIPA concept particularly attractive in practice. The flexibility and robustness of the procedures were confirmed by Monte Carlo simulations.

# 4. Collective Approach to High Frequency Transmission of Electromagnetic Waves Through Dielectric Layers

Professor L.B. Felsen and Mr. P.D. Einziger

Transmission through layered media is of interest for various applications in electromagnetics and optics. Examples are provided by curved dielectric radome covers for microwave antennas, and by layered optical filters. A common approach to this problem, when the excitation comes from a realistic localized source, is to trace rays successively through the layered structure. Due to internal reflections at the layer interfaces, this procedure gives rise to a multiplicity of ray fields, which renders computation inconvenient and physical interpretation awkward.

By a novel approach, based on selective Poisson summation of the above-noted ray fields, we have managed to treat higher-order multiple internal reflection events in a collective manner. One thereby obtains a representation for the transmitted field comprised of a certain number N of ordinary ray fields with internal reflections  $0 \le n \le N$ , plus a "collective" ray field with weighted amplitude that accounts for all orders of reflection n > N. The collective weighting incorporates composite plane wave transmission coefficients for the equivalent local layer structure (with previously ignored curvature corrections for nonplanar layers) rather than the transmission and reflection coefficients for a single interface, which appear in the ordinary ray fields. The number N of ordinary rays must be large enough so that all rays with n > N exhibit the phase coherence descriptive of local plane wave transmission. For relatively thin layers, the collective ray concept is found to be valid even for the direct ray path without internal reflect tions so that the entire source-excited transmitted field is represented accurately by a single species of collective rays.

"Collective ray optics" may be regarded as a generalization of conventional ray optics for layered media. The validity of the field formulation in terms of ordinary and collective rays has been verified by comparison with independently derived results for the rigorously solvable prototype of a circular cylindrical layer of constant thickness. The investigations so far have been restricted to line-source-excited two-dimensional configurations. Extensions to other source types (discrete and continuous aperture distributions) and to three-dimensional structures, with emphasis also on polarization effects, are planned for the future.

# 5. Optimal Multivariable Controllers Employing a Two-Degree-of-Free-dom Design Methodology

Professors D.C. Youla and J.J. Bongiorno, Jr.

By and large, the design of optimal Wiener-Hopf controllers for linear large-scale time-invariant plants has been restricted to one-degree-of-freedom control laws. In turn, this has practically precluded

the use of reduced-order modeling and has made it impossible to adequately incorporate other "hard" design specifications imposed by sensitivity constraints and phase-gain stability margin requirements into a bonafide optimality theory. The conventional single-loop configuration satisfies the required closed-loop stability, but forces the rejection of other solutions which, although they could provide performance better than an order of magnitude, are inconsistent with single-loop stability.

Guided and motivated by the desire to control large-scale systems simply and effectively, we have reexamined these previously-rejected solutions and have discovered that the potential of some of those solutions can be realized, consistent with system stability, if the topology of the control structure is appropriately altered to include suitable minor-loop feedback. Using this approach, we have developed a two-degree-of-freedom design methodology. By exploiting the additional degree of freedom, it has been possible to combine transient and steady-state performance requirements with "hard" constraints imposed by sensitivity and stability margins. In some cases we have obtained an improvement of two orders of magnitude over the more conventional one-degree-of-freedom design techniques! The possibilities appear exciting but further research is necessary before a complete theory becomes available.

# 6. New Interpretation of Size Effects in the Conduction Properties of Thin Metallic Films.

Professor H.J. Juretschke and Mr. R. Pimpinella

Size effects describe the influence of surface scattering of conduction electrons on the conductance of thin metallic films. If properly understood, they contain information about the environment in the surface region sensed by these electrons. We have proposed a new interpretation of size effects that is based on the proposition that the so-called surface scattering actually takes place throughout a small but finite layer of the solid just beneath the geometrical surface, rather than being due entirely to the geometrical features of the surface boundary itself, as has been commonly assumed. The theory has been formulated in terms of two principal parameters that define the properties of the scattering layer: its thickness and the surface region mean-free path. It incorporates contributions to the surface mean-free path arising both from a modified surface phonon spectrum and from static structural disorder. Most of the results of current models for size effects are either contained in our formulation, or are mimicked by it, though for different underlying reasons. The theory has so far been very successful in three different applications: (a) the surface scattering by clean and smooth metal surfaces over a large range of temperatures, (b) the influence of surface charge on this surface scattering, and (c) the scattering by controllably produced very thin rough overlays on the same originally very smooth surface. The results of this interpretation imply that well-annealed metal surfaces have a characteristic domain structure of atomically smooth regions separated by extended faults, rather than disorder on the scale of individual atoms.

# 7. Leaky Wave Theory for Dielectric Grating Antennas of Finite Width

# Professors S.T. Peng and A.A. Oliner

An important class of antennas for millimeter waves, on which much experimental effort has been conducted during the past half-dozen years in various laboratories around the world, consists of a periodic grating cut into the top of dielectric image guide. The period of the grating relative to that of the wavelength is such that the n=-1 space harmonic of the wave guided along the dielectric image guide radiates power away from the guide at some angle, thereby changing the formerly bound mode into a leaky mode. The dielectric image guide is simply a rectangular dielectric strip placed on a metal ground plane, so that the grating antenna promprised of periodic grooves on the top of that dielectric strip, is simple in form, easy to fabricate, and suitable for inclusion in a millimeter wave integrated circuit.

Until our recent work, no theory was available which could permit one to compute the leakage properties of such grating antennas of finite width, and therefore permit such antennas to be designed in a systematic way. Our theory makes use of a solution for the oblique guidance of electromagnetic surface waves by periodically grooved dielectric layers. That basic solution was reported by us last year as a new canonical result of potential importance in many applications; this is one of them. The oblique guidance arises because the dielectric image guides, and therefore the gratings placed on them, are necessarily of finite width. Our theory now makes it possible to systematically design this new class of millimeter wave antennas.

# 8. <u>Direct Phase Determination of X-ray Structure Factors Using</u> Reflected Intensities in the Renninger Geometry

### Professor B. Post

The long-known Renninger effect (where by rotation of a crystal around the normal to planes in reflecting position, various other planes are simultaneously brought into reflecting conditions, resulting in significant changes in reflected intensity) has been carefully reexamined with respect to information on the phase of x-ray structure factors. Our earlier success in the identification of phase information in the experimental results of the multiple-beam Borrmann effect - the anomalous transmission of x-rays through crystals - and in understanding the causes for the phase sensitivity, have enabled us to pinpoint where the corresponding effects should occur in the reflection geometry of the Renninger effect: The wings of the Renninger peaks or dips must show left-right asymmetry. These predictions have been verified by focusing on the intensity variations around n-beam couplings near the base line provided by the reference reflection.

We have been able to identify literally hundreds of phases of x-ray reflections in a variety of crystals, all in agreement with the phases that had been found earlier by indirect means. The crystals ranged

from highly perfect to moderately mosaic, from highly transmitting to heavily absorbing, and the basic reflections included those of both large and small structure factors.

As a result of this study, it is clear that experimental phase information is readily available in the reflection geometry of the Renninger effect, and under relatively simple instrumental constraints.

# 9. Theory of Phase Information of X-ray Structure Factors in the Asymptotic Intensities Near n-Beam Interactions

Professor H.J. Juretschke

Post's recent work has shown that the <u>asymmetry</u> of the observed integrated intensity of a Bragg reflection in the immediate neighborhood of many 3-beam or higher-order-beam interactions can be directly tied to the <u>sign of the phase</u> of the structure factors involved in that interaction. As a consequence, it has become important to be able to refer to a simple and practical guide for identifying those interactions that lend themselves to optimal phase determinations, relative to angular resolution, as well as to magnitude of the effect.

Such a theoretical guide has been developed on the basis of dynamical theory, using a perturbation theory approach with respect to the influence of the additional interactions on basic reflection. Perturbation theory establishes that to first order the additional interactions manifest themselves in a simple asymmetric modification of the original 2-beam diffraction structure factor, leading to an increase in integrated intensity on the other side. The direction of this change is determined by the phase of the structure factor combination characterizing this interaction.

The theory for a symmetric reflection shows that these effects are different for the two polarization states of x-rays, and in each case it yields a fully quantitative measure of the asymmetry as a function of the strengths of all the structure factors involved and of the geometrical relations between the propagation vectors of all the active wavefields. Furthermore, the asymptotic theory automatically includes the interpretation of 4-beam and higher interactions.

One of its most important features, from the point of view of significant application, is that its formalism is readily applicable to the determination of phases in noncentrosymmetric crystals. This requires a quantitative examination of the degree of asymmetry in the intensities in the opposite wings of the interaction peak. Obviously, such a quantitative interpretation can only be successful if experiments can be carried out within certain requirements of precision. The formulas of the asymptotic theory provide first order bounds on angular resolution and monochromaticity, and especially indicate the need for using polarized incident beams, and polarization-sensitive detectors for an accurate analysis of the phase-dependent data.

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